

Particle acceleration at travelling shocks in the heliosphere

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Abstract

The acceleration of energetic protons from the solar wind (SW) distribution by travelling interplanetary shocks is investigated. The SW velocity distribution is represented using kappa functions, which are transformed in response to simulated shock transitions in the plasma flow speed, number density, and temperature. These heated SW distributions are specified as a particle source at shocks from which particles with sufficient energy can be injected into the diffusive shock acceleration (DSA) process. DSA is modelled within the context of the Parker transport equation, which is solved using time-backward integrated stochastic differential equations. Two broad applications are considered: firstly, the acceleration of particles at fast-moving interplanetary shocks driven by coronal mass ejections (CMEs), and secondly, the acceleration of particles at the compression waves bounding corotating interaction regions (CIRs). For CME-driven shocks, it is shown that the maximum attainable energies of shock-accelerated spectra are limited by the shocks' transit times, while spectra may be accelerated to higher energies in the presence of enhanced magnetic turbulence or at faster-moving shocks. Indeed, simulations suggest fast-moving shocks are more likely to produce very high-energy particles, while strong shocks, associated with harder shock-accelerated spectra, are associated with higher intensities of energetic particles. The prior heating of the solar wind distribution is found to complement shock acceleration in reproducing the intensities of typical energetic storm particle (ESP) events, especially where injection energies are high. Moreover, simulations of 0.2 to 1 MeV proton intensities are presented that reproduce the observed flat energy spectra prior to shock passages, owing to the modulation of low-energy particles. Whereas spectra adhering to the predictions of DSA are usually indicative of local acceleration, the modulation of spectra at low energies emerges as a recurring signature of particles transported to the observer from remote acceleration sites. In these cases, magnetic connections are important for particle transport between the shock and the observer, especially where the observer is not in the direct path of the shock, whereas perpendicular diffusion becomes more important when magnetic connections are absent. At CIRs, accelerated particle intensities consistently peak near the trailing edge. These peak intensities scale proportional to local compression ratios, but only if energy distributions display the features of DSA, which ostensibly occurs when particles are accelerated locally. By contrast, when accelerated spectra are appreciably modulated, which is likely indicative of an increased proportion of remotely accelerated particles, no correlation is found between peak intensities and local compression ratios. DSA is demonstrated to reproduce many of the salient features of ESPs and CIR particles, highlighting its prevalence as an acceleration mechanism at interplanetary shocks. As a source population, the heated SW distribution makes an important contribution in this regard, providing large numbers of adequately energized seed particles for DSA to reproduce typical energetic particle intensities.

Keywords:

energetic particle transport, interplanetary shocks, diffusive shock acceleration, coronal mass ejections, corotating interaction regions, solar wind, stochastic differential equations, heliosphere.

Acronyms and Abbreviations

2D	Two Dimensional
3D	Three Dimensional
AU	Astronomical Unit
CME	Coronal Mass Ejection
CIR	Corotating Interaction Region
DSA	Diffusive Shock Acceleration
ESP	Energetic Storm Particle
FLS	Fast Latitude Scan
HMF	Heliospheric Magnetic Field
MFP	Mean Free Path
MHD	Magnetohydrodynamic
SDE	Stochastic Differential Equation
SEP	Solar Energetic Particle
SI	Stream Interface
SIR	Stream Interaction Region
SW	Solar Wind
TPE	Transport Equation

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Chapter 1

Introduction

Energetic particle events are often observed during the passages of interplanetary shocks, driven either by coronal mass ejections (CMEs) or associated with corotating interaction regions (CIRs). Diffusive shock acceleration (DSA) is widely regarded as the most plausible mechanism for accelerating particles during the aforementioned events [*e.g. Desai and Giacalone, 2016; Richardson, 2018*]. The solar wind (SW), meanwhile, is arguably the most ubiquitous source of ionized particles in the inner heliosphere. In this study, the energy distribution of SW particles is considered in two ways: thermodynamically, as it relates to its transformation in response to changing SW conditions during shock passages, and as a source from which particles may be accelerated by the aforementioned travelling shocks. This acceleration process is simulated by means of solving stochastic differential equations (SDEs) that are equivalent to the *Parker* [1965a] transport equation (TPE).

Two broad applications are considered: simulating energetic storm particle (ESP) events, associated with the passage of CME-driven shocks, and the acceleration of particles in CIRs. The investigations in this study are centred about the following broad scientific themes:

- the manifestation of the classical features of DSA in the energy distributions of particles accelerated during ESP and CIR events,
- the contributions to intensities, as viewed by a particular observer, from particles accelerated *locally* (that is, at the observer's location at the time of the shock's arrival) versus those accelerated *remotely* and subsequently transported to the observer, and
- the role of the SW distribution as a source of seed particles for DSA during ESP and CIR events.

The study is structured within this thesis as per the chapter divisions discussed below:

Chapter 2 introduces content that is pertinent as background to the rest of the study. This includes introductory discussions on solar activity, collisionless shocks, and energetic particles in the inner heliosphere. Important assumptions regarding the SW and the heliospheric magnetic field are also discussed here. Furthermore, a concise introduction to various conceptual aspects of DSA is provided. The SW energy distribution and its representation using kappa functions are also discussed.

Chapter 3 provides the theoretical background for modelling particle transport and shock acceleration. This chapter introduces the distribution function and the *Parker* [1965a] TPE, and discusses the representation of each of the considered physical processes in the TPE. This chapter also introduces SDEs. Details are provided regarding the general formulation of the SDEs, as well as their numerical implementation, limitations, and advantages. Finally, a proof-of-concept model is introduced to illustrate the features of DSA for a simple transport configuration, along with an importance sampling technique that could potentially improve the numerical efficiency of SDE simulations.

The acceleration of SW particles at CME-driven shocks is investigated in **Chapter 4**. For this application, a spherically symmetrical model configuration is introduced. The shock transitions of SW quantities, and the consequent shock-driven transformation of the SW energy distribution, are discussed. This chapter furthermore explores how particles accelerated at CME shocks display the spectral characteristics of DSA, how the efficiencies of fast and strong shocks compare, and lastly, how particles may be accelerated from the SW distribution to typical ESP energies. As part of this section, the evolution of the spatial and spectral features of particles accelerated throughout the transit of the shock is discussed. The contents of this chapter are largely based on results published in *Prinsloo et al.* [2019].

Chapter 5 serves as a transition chapter, introducing concepts relevant to the multidimensional particle transport considered in the next chapter. Here, the model introduced in the previous chapter is adapted to include two spatial dimensions, and a simple illustrative description for a 2D CME shock is introduced. This chapter discusses how the transport of accelerated particles is affected by the longitudinal extents of CME shocks and by varying levels of diffusion parallel and perpendicular to magnetic field lines. These effects are considered from the perspectives of observers both in and outside of the direct paths of travelling shocks.

The shock acceleration and transport of particles in CIRs are investigated in **Chapter 6**. For this chapter, an analytical description of CIRs is introduced to simulate the features of SW quantities associated with these structures. Furthermore, it is discussed how changes in these SW quantities affect the transformation of the SW distribution during the passage of the CIR. Several aspects of the modelling process are revisited, especially those aspects that differ substantially from how acceleration at CME shocks is modelled in previous chapters. Among these is the introduction of a new spatially dependent model for the injection of particles into the DSA process inside CIRs. Simulated time-intensity profiles and energy spectra of CIR particles are presented. The organization of these particles' intensities and the sites of their acceleration are discussed at length.

Finally, **Chapter 7** concludes by discussing the main results of the study in the context of the broad scientific themes listed above, and briefly outlines avenues for future research.

Chapter 2

On energetic particles, shocks, and the heliosphere

2.1 Introduction

This chapter briefly introduces pertinent concepts as background for the rest of the study. These concepts include the heliosphere and solar wind (SW), their variation with the solar activity cycle, and the heliospheric magnetic field. Also discussed are events such as coronal mass ejections (CMEs) and the formation of corotating interaction regions (CIRs). The shocks associated with these heliospheric phenomena are of particular interest as they are thought to be responsible for accelerating energetic particles. A concise explanation of the mechanism by which these particles may be accelerated at shocks is given. Finally, the SW velocity distribution, as a source from which particles may be accelerated, is discussed.

2.2 The near-Earth heliosphere and solar variability

The outer atmosphere of the Sun, or solar corona, must continually expand into interplanetary space to maintain hydrodynamic equilibrium [Parker, 1958, 1965b]. This coronal expansion forms the SW, which creates a cavity in the interstellar medium filled with ionized solar plasma. This cavity is referred to as the heliosphere. In the approximate direction of its own movement, the heliosphere extends up to $r \sim 120$ AU from the Sun, as initially revealed by Voyager 1, and recently confirmed by Voyager 2 during the second *in situ* sampling of interstellar space by a spacecraft. See the summary by Strauss [2019] and the references therein.

Since the events of interest in this study are those affecting the near-Earth environment, only the first ~ 5 AU from the Sun is of importance. The present study is furthermore limited to regions outside of the solar Alfvén radius r_A (typically several solar radii from the Sun), where the energy density of the SW flow exceeds the magnetic energy density [e.g. Gary, 2001]. In this region, the SW expands at supersonic proton speeds between ~ 400 and 800 km s^{-1} and carries out the *frozen-in* solar magnetic field into interplanetary space. This outflow forms the heliospheric magnetic field, which is embedded in the plasma flow owing to the large electrical

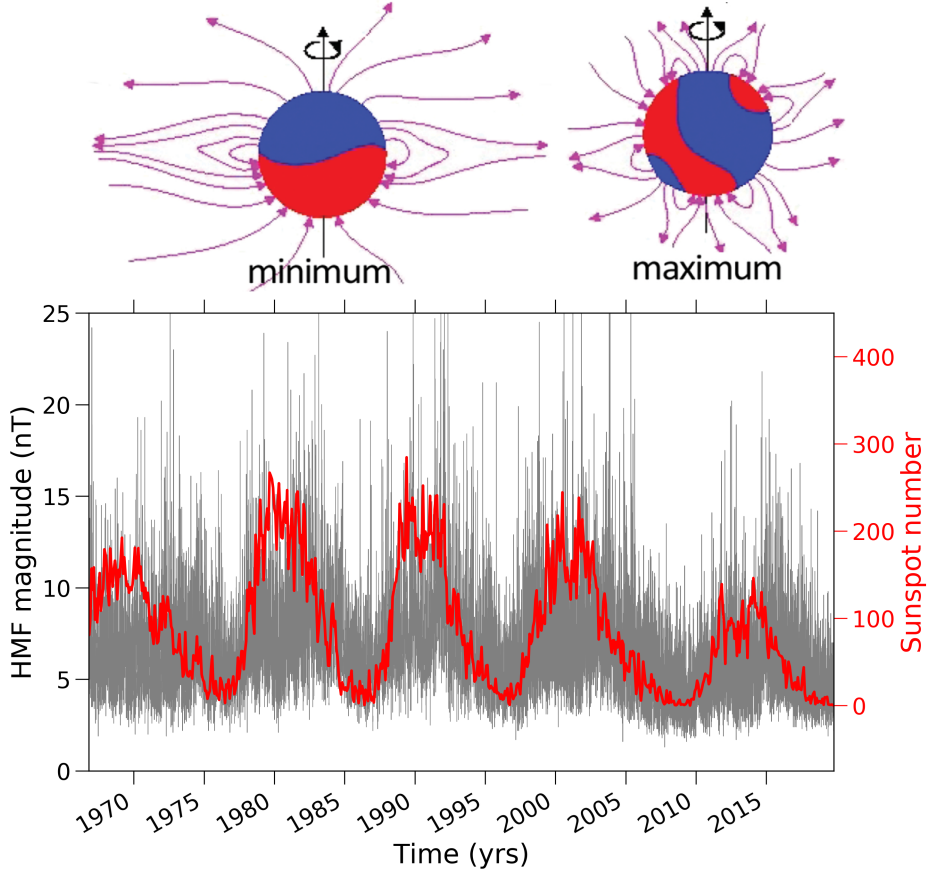


Figure 2.1: Top: Artist renditions [adapted from *Heber and Potgieter, 2006*] of the solar magnetic field during solar minimum and maximum conditions as shown on the left and right, respectively. Bottom: Time series of the daily-averaged heliospheric magnetic field (HMF) magnitude measured by ACE/IMP8 (shown in grey), and the monthly-averaged sunspot number (shown in red). Both quantities adhere to the 11-year solar activity cycle. The magnetic field data is obtained from NASA SPDF COHWeb, and the sunspot data from the World Data Center SILSO, Royal Observatory of Belgium, Brussels.

conductivity of the SW. The heliospheric magnetic field is typically described in this study using the *Parker [1958]* field model.

By contrast, at $r < r_A$ in the corona, the magnetic field dominates the plasma flow [e.g. *Gary, 2001*]. This results in the formation of coronal holes where open magnetic field lines facilitate the outflow of solar plasma, which in turn results in fast SW streams emanating from these coronal holes. The solar magnetic field varies according to the 11-year solar activity cycle as illustrated in Figure 2.1. The top panel of this figure shows that, when the Sun is active, the magnetic field displays a less-defined structure. As a result, the distribution of coronal holes would be largely random. This is illustrated in Figure 2.2, which shows *Ulysses* spacecraft observations taken during different phases of the solar activity cycle. The bottom panel shows that the positions of fast SW streams exhibit no discernible heliographic latitude dependence during solar maximum conditions, but are distributed randomly. However, during solar minimum, field lines near the poles are typically open, facilitating the development of fast SW streams, with speeds of $\sim 800 \text{ km s}^{-1}$, emanating from large polar coronal holes [*Phillips et al., 1995*]. The top panel of Figure 2.2 shows the enhanced flow speeds that emerge at high heliographic latitudes during solar minimum conditions. As discussed in Section 2.2.2, these fast SW streams are involved in the formation of CIRs.

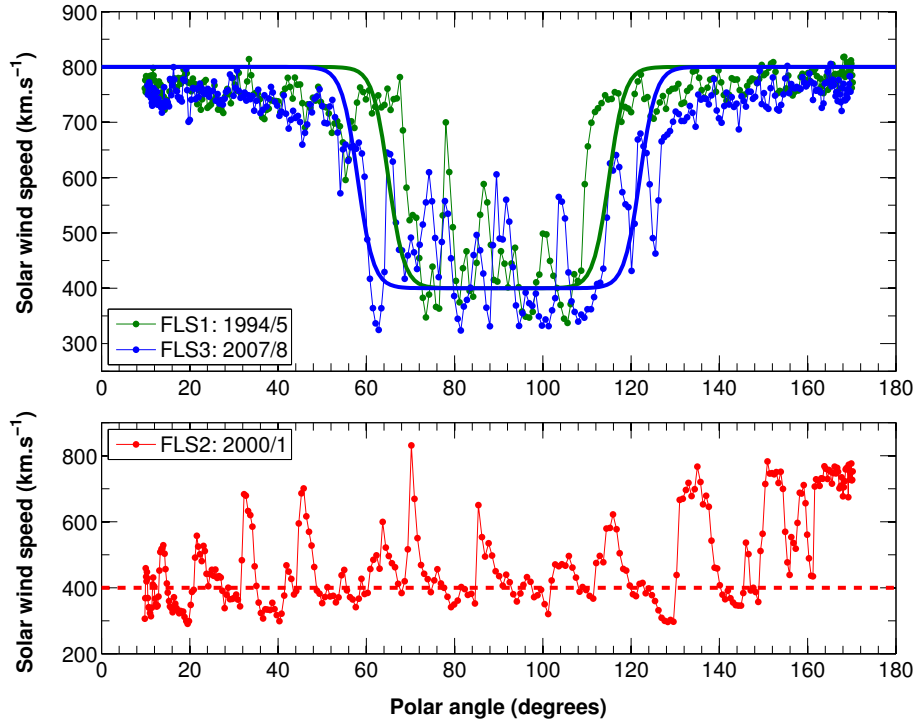


Figure 2.2: SW speed as a function of heliographic latitude. The top and bottom panels show Ulysses observations taken during solar minimum and maximum conditions, respectively. Each set of measurements, presented in different colours, refers to the Fast Latitude Scan (FLS) corresponding to the dates given in the figure legends. The line-connected markers represent spacecraft measurements. The thick solid lines in the top panel are fits to these measurements, whereas the dashed line in the bottom panel indicates the average slow SW speed. Data obtained from NASA SPDF COHWeb.

The bottom panel of Figure 2.1 also shows the variation of sunspot numbers with time. Sunspot numbers are commonly used as proxies for solar activity and are related to the number of dark, irregularly shaped blemishes that are visible on the Sun’s photosphere (the lower solar atmosphere from which light radiates). Their dark appearance likely follows from the repulsion of surrounding plasma by strong magnetic fields. Magnetic field lines form coronal loops between sunspot groups, which often form part of active regions that are associated with solar transient events, such as flares and CMEs. CMEs are of particular interest and are discussed further below. For more information regarding sunspots, and how they are quantified, refer to *Hoyt and Schatten [1998]* and *Clette et al. [2014]*.

The following discussions give only a brief overview of the SW and magnetic properties associated with CMEs and CIRs. Detailed descriptions of these quantities are provided as required for each application in later chapters.

2.2.1 On coronal mass ejections

During CMEs, large quantities of solar coronal plasma are released into interplanetary space. Given their association with active regions on the Sun, CMEs are more frequent during solar maximum conditions. Although CMEs and solar flares are often observed concurrently with a well-established statistical relationship, they may occur independently, and their physical relationship remains the subject of ongoing study [*Suryanarayana, 2019; Moschou et al., 2019; Firoz*

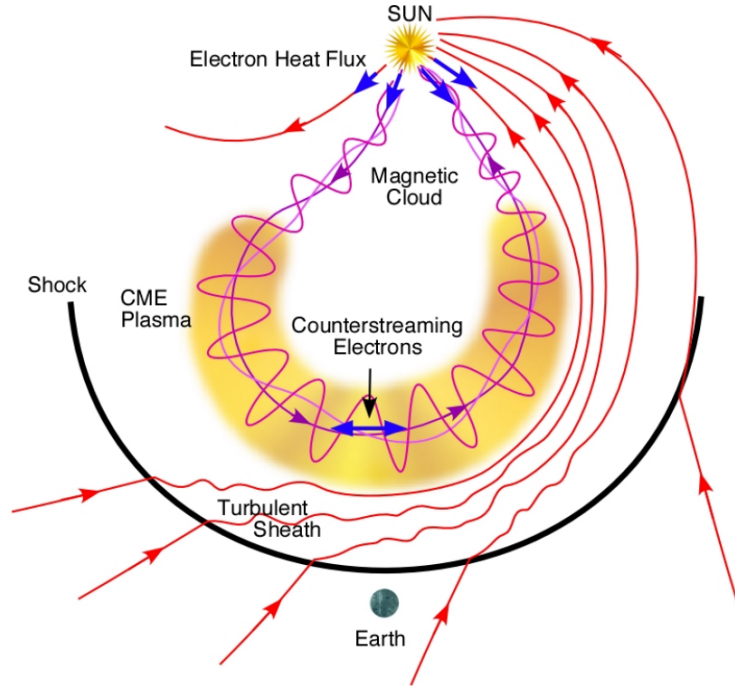


Figure 2.3: Schematic by Zurbuchen and Richardson [2006] of a CME propagating into interplanetary space, depicting the ejected coronal plasma, borne by flux ropes, and the shock front (indicated by the solid black line) driven ahead of a turbulent sheath region. Magnetic field lines are shown in red.

et al., 2019]. The properties of CMEs during their propagation into interplanetary space also appear to depend on their early development near active regions [Pal *et al.*, 2018]. CMEs may be described as the eruption of coronal flux ropes [Chen *et al.*, 1997, 2000], which are essentially bundles of helical magnetic field lines along which coronal plasma is transported, as depicted in Figure 2.3. Originating in the corona, their eruption is accompanied by the dissipation of large amounts of magnetic energy, which presumably provides the energy for their propagation. CMEs propagating outward in interplanetary space are distinguishable from the ambient SW by their own plasma and magnetic signatures [e.g. Zurbuchen and Richardson, 2006]. The region in the wake of the CME's leading edge is characterized by enhanced and smooth magnetic fields with rotating components, which are distinctive properties of magnetic clouds [Klein and Burlaga, 1982; Burlaga *et al.*, 1982], whereas a compressed sheath region with enhanced magnetic turbulence is typically observed ahead of it [e.g. Kilpua *et al.*, 2017]. These regions are also illustrated in Figure 2.3.

Owing to their fast propagation speeds, shocks may form ahead of CMEs. Interplanetary CMEs driving shocks that are capable of producing energetic particles are of particular interest to the present study. Events during which the intensities of energetic ions and electrons are enhanced, concurrent with the passage of CME-driven shocks, are often referred to as ESP events [Bryant *et al.*, 1962; Lario and Decker, 2002; Ho *et al.*, 2009; Huttunen-Heikinmaa and Valtonen, 2009]. These events typically involve halo CMEs that drive fast shocks [Lario *et al.*, 2005b] with concomitant observations of type II radio emissions, but not without exceptions [e.g. Mäkelä *et al.*, 2011]. Furthermore, the seed particles for ESP events are thought to be sourced from either the thermal or suprathermal SW [Gosling *et al.*, 1981; Lee, 1983; Baring *et al.*, 1997] or solar energetic particles (SEPs) produced in flares [Tan *et al.*, 1989; Li *et al.*, 2014]. See also the discussions by Desai and

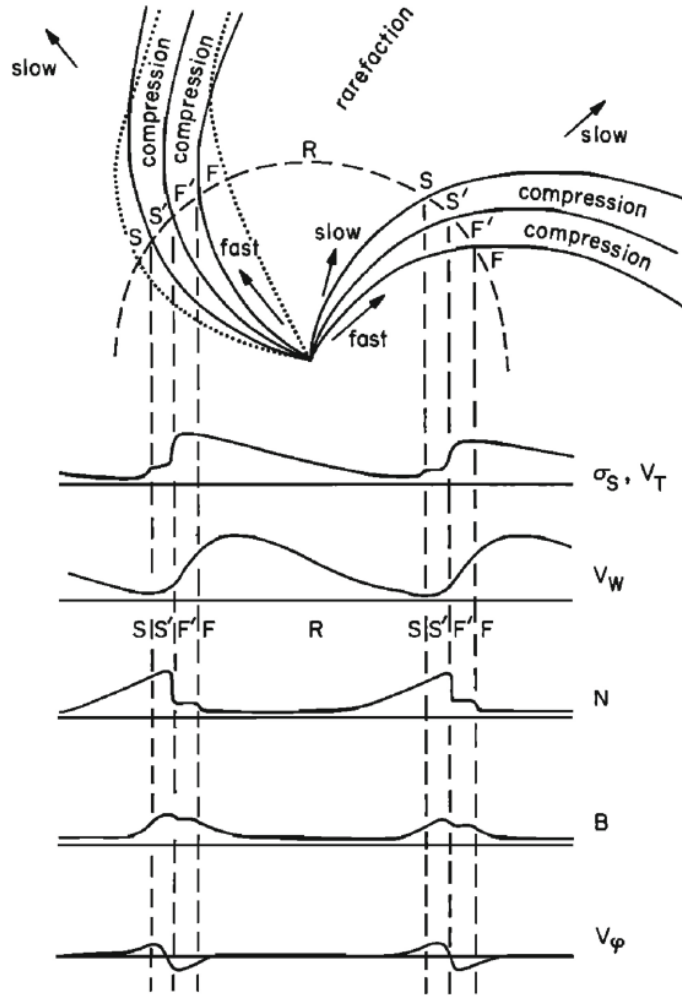


Figure 2.4: Schematic by *Belcher and Davis* [1971] of two fast SW streams forming CIRs in their interaction with the ambient slow SW, along with profiles illustrating the various SW quantities in the different flow regions inside the CIRs. These SW quantities (from the top to the bottom) are the thermal speed (V_T , related to SW temperature) or the level of magnetic field fluctuations (σ_S), the SW flow speed, number density, magnetic field magnitude, and transverse SW flow components. The flow regions labeled S and F are the unperturbed slow and fast SW streams, whereas S' and F' represent their compressed counterparts. The S - S' , S' - F' , and F' - F boundaries are the leading edge, stream interface, and trailing edge of the CIR, respectively.

Giacalone [2016] on CMEs and ESPs.

2.2.2 The formation of corotating interaction regions

When coronal holes extend to low heliographic latitudes, the associated fast SW streams may overtake the slow SW emitted from the Sun at an earlier time. Owing to the rotation of the Sun, these fast and slow SW flow regions become radially aligned and interact to form compression regions that co-rotate with the Sun [*e.g. Gosling, 1996*]. These are known as CIRs.

As illustrated in Figure 2.4, regions of distinct flow characteristics emerge as a result of the interaction between the slow and fast SW streams and are separated by at least three boundaries [*Belcher and Davis, 1971*]. At the interaction region, both slow and fast streams are compressed, and the former is accelerated at the leading edge, while the latter is decelerated at the trailing

edge of the CIR. Furthermore, the compressed slow and fast flow regions are separated by the stream interface. Owing to the fact that the frozen-in magnetic fields in the two plasmas cannot interpenetrate, plasma flows on either side of the stream interface are deflected in opposite directions. These deflections are visible in Figure 2.4 as transverse flow speed components on either side of this boundary. Moreover, the SW density in the interaction region at least roughly appears to be inversely proportional to the flow speed. In particular, this manifests as a broad rarefaction region in the fast stream beyond the trailing edge. The SW plasma and magnetic properties are revisited in more detail in Chapter 6.

As discussed in Section 2.3, shocks may form at both edges of the CIR. These shocks can accelerate particles to MeV energies [Barnes and Simpson, 1976; Fisk and Lee, 1980]. In fact, since ESPs and SEPs are accelerated by either CME-driven shocks or solar flares, and these events are more commonplace during active solar conditions, CIRs are the primary acceleration site for energetic particles during solar minimum [e.g. Richardson *et al.*, 1993]. The source population for these CIR particles is most often based in the high-energy tails of SW distributions [Mason *et al.*, 2008, 2012; Bučík *et al.*, 2012; Filwett *et al.*, 2017; Yu *et al.*, 2017, 2018]. However, SEP events may also on occasion provide seed particles for acceleration at CIRs [e.g. Bučík *et al.*, 2011].

Sections 2.3 to 2.5 discuss the typical properties of the shocks associated with interplanetary CMEs and CIRs, the likely mechanism for the acceleration of ESPs and CIR particles, as well as the potential SW-based source of their seed particles.

2.3 Travelling shocks in the inner heliosphere

Shocks in astrophysical environments are characterized by magnetized and dilute media, and are often collisionless [e.g. Stockem Novo *et al.*, 2016], implying that energy is dissipated by means of interactions between particles and magnetic fields (or waves propagating along magnetic fields) rather than inter-particle interactions. This is also valid for shocks in the SW.

Shocks move faster than any wave mode in the medium that can transfer information that may forewarn of their arrival. In the SW, disturbances propagate as magnetosonic waves. Therefore, restoration forces opposing displacements by waves propagating in the SW may stem from either pressure gradients or magnetic stresses. These waves are referred to as fast or slow mode waves depending on whether the aforementioned forces act in or out of phase, respectively [Choudhuri, 1998]. Simply stated, such waves may form shocks if they propagate faster than the restorative forces can act to restore the changes imposed by the waves. Fast and slow-mode magnetosonic waves steepen into shocks when the upstream (downstream) plasma flow speed in the shock frame is larger (smaller) than the local magnetosonic phase speed, given by [e.g. Kallenrode, 1998]

$$2v_{F,S}^2 = (v_A^2 + v_s^2) \pm \sqrt{(v_A^2 + v_s^2)^2 - 4v_s^2v_A^2 \cos^2 \Theta_{BN}}, \quad (2.1)$$

where the + and – signs correspond to the fast (F) and slow (S) mode phase speeds, respectively. The quantities $v_A = B/\sqrt{\mu_0\rho}$ and $v_s = \sqrt{\gamma_c P/\rho}$ are the respective Alfvén and sonic speeds, with B the magnetic field magnitude, ρ the mass density, P the proton pressure, γ_c the ratio of specific heats, μ_0 the permeability of free space, and Θ_{BN} the angle between the

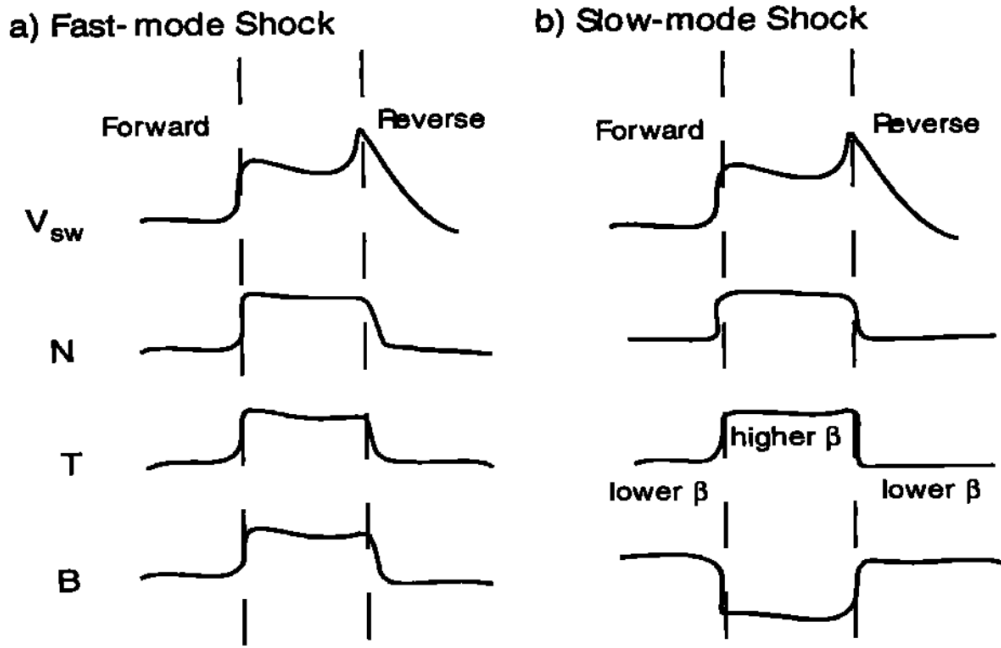


Figure 2.5: Schematic from *Ho et al.* [1998] illustrating how plasma properties change across pairs of forward and reverse fast-mode shocks (shown on the left) and slow-mode shocks (shown on the right). The profiles as shown from the top to the bottom are the SW flow speed in the spacecraft frame, number density, temperature, and magnetic field. The plasma- β parameter refers to the ratio of plasma pressure to magnetic pressure.

shock normal and the magnetic field. Furthermore, for fast-mode shocks, both the up and downstream flow speeds (in the shock frame) exceed v_A , whereas the upstream flow speed at slow-mode shocks exceeds the sound speed, but remains sub-Alfvénic [*Ho et al.*, 1998; *Kallenrode*, 1998].

Interplanetary shocks are typically fast-mode shocks, with few exceptions [*Richter*, 1991; *Ho et al.*, 1998; *Zuo et al.*, 2006]. In the corona, slow shocks are more commonplace [e.g. *Hundhausen et al.*, 1987], because both v_s and v_A are larger. A notable difference between the two shock modes is that the magnetic field jumps in the same direction as the other SW quantities across the fast-mode shocks, but in the opposite direction across the slow-mode shocks [e.g. *Ho et al.*, 1998; *Lepping*, 2000]. This is illustrated in Figure 2.5. The forward and reverse descriptors refer to the direction of the shocks' propagation in the SW frame, where a forward shock propagates towards the Sun, and a reverse shock propagates away from it. The enhanced plasma- β parameter inside the interaction region formed by the pairs of slow-mode shocks in Figure 2.5 indicates that the plasma pressure between the shocks is enhanced relative to the magnetic pressure, which is consistent with the lowered magnetic field.

The obliquity of a shock is described in terms of Θ_{BN} as defined for Eq. 2.1. A parallel shock, with $\Theta_{BN} = 0$, propagates parallel to the magnetic field, and its normal is therefore directed along the magnetic field. On the other hand, a perpendicular shock, with $\Theta_{BN} = 90^\circ$, propagates perpendicular to the magnetic field, and has a normal that is orthogonal to the magnetic field. Oblique shocks can be further categorized as quasi-parallel for $0 < \Theta_{BN} < 45^\circ$ or quasi-perpendicular for $45^\circ < \Theta_{BN} < 90^\circ$. Note that the component of the magnetic field along the shock normal does not change across the shock [e.g. *Kallenrode*, 1998], implying that the tangen-

tial component must increase when the magnetic field magnitude increases across a fast-mode forward shock. In this case, field lines bend away from the shock normal. Similarly, field lines bend toward the shock normal when the magnetic field decreases across a slow-mode forward shock. Note that for $\Theta_{BN} = 90^\circ$, the fast and slow-mode phase speeds follow from Eq. 2.1 as $\sqrt{v_A^2 + v_s^2}$ and zero, respectively. Perpendicular shocks are fast-mode shocks, since slow-mode shocks do not propagate orthogonal to the magnetic field [Boyd *et al.*, 2003].

Interplanetary CME-driven shocks are typically fast-mode forward shocks [Lario *et al.*, 2005b; Ho *et al.*, 2008] and vary in obliquity with time and longitude [e.g. Zank *et al.*, 2006; Hu *et al.*, 2017]. However, whereas an idealized smooth shock may vary from being quasi-perpendicular to quasi-parallel from one CME flank to another, realistically, the shock front may be rippled so that local geometries may resemble any obliquity [see Klein and Dalla, 2017]. The CME shocks considered in the present study are assumed to have smooth shock fronts with shock normals directed in the radial direction. Under this simplification, the obliquity may be inferred from the winding angle of the Parker [1958] spiral.

The shocks associated with CIRs may occur as pairs of forward and reverse shocks (as shown in Figure 2.5), and, as mentioned before, only occasionally tend to be slow-mode shocks [e.g. Ho *et al.*, 1998]. Shocks bounding CIRs tend to form at larger radial distances [$r \gtrsim 2$ AU, Gosling *et al.*, 1976; Hundhausen and Gosling, 1976; Smith and Wolfe, 1976] and are seldom observed at 1 AU [Jian *et al.*, 2006]. This is owing to the fact that the sonic and Alfvén speeds, on which the magnetosonic speeds in Eq. 2.1 depend, decrease with increasing distance from the Sun. Since CIRs propagate at fixed speeds related to the solar rotation rate, the decrease in the speeds of the acoustic and magnetic waves that may forewarn of magnetosonic disturbances is necessary for the compression waves at the leading and trailing edges of CIRs to steepen into shocks. This steepening process and the obliquity of CIR shocks are revisited in Chapter 6.

2.4 Diffusive shock acceleration

Diffusive shock acceleration [DSA; Axford *et al.*, 1977; Krymskii, 1977; Bell, 1978a, b; Blandford and Ostriker, 1978] is a well-known mechanism for accelerating energetic particles at shocks associated with interplanetary CMEs or CIRs. This section gives a concise conceptual introduction to this acceleration mechanism, whereas its features are discussed in greater detail within the context of simulations in subsequent chapters. See also Vainio [1999] and the relevant discussions of Desai and Giacalone [2016] and Li [2017] for more on DSA.

2.4.1 A conceptual introduction

DSA involves particles gaining energy during a process where they are repeatedly scattered across shocks by means of their interactions with scattering centres. In the SW, these scattering centres may be thought of as irregularities in the frozen-in magnetic field, Alfvén waves propagating along or perpendicular to the magnetic field, or even magnetic mirrors [e.g. Giacalone

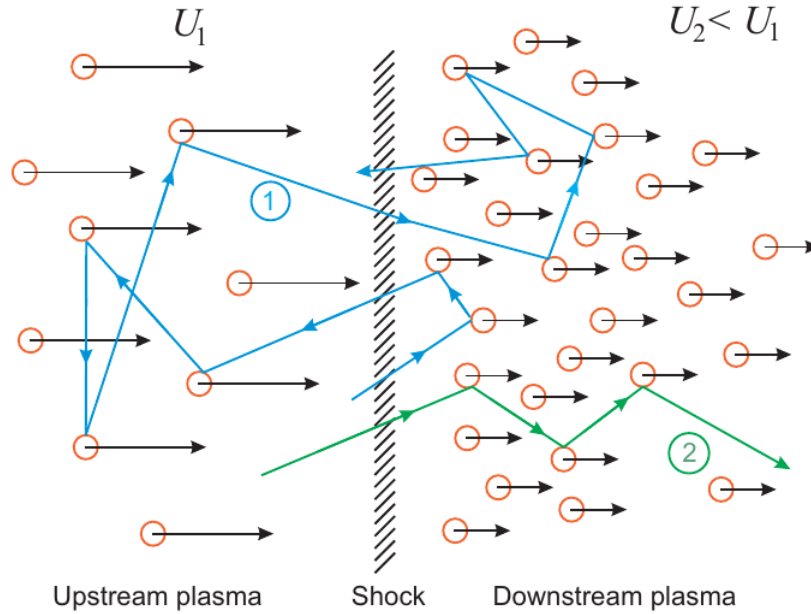


Figure 2.6: Schematic by *Achterberg* [2008] illustrating the DSA mechanism for particle acceleration. The upstream and downstream flow speeds, in the rest-frame of the shock, are denoted U_1 and U_2 , respectively, with $U_2 < U_1$. Circles represent scattering centres, while black arrows indicate their direction of movement. The blue and green trajectories, labelled 1 and 2, respectively, give examples of how particles may interact with scattering centres.

et al., 2002]. In terms of particle transport, this scattering process may be described using diffusion coefficients, where small coefficients imply stronger scattering. Whereas DSA functionally entails the energy gain of an ensemble (or distribution) of particles having completed multiple scattering cycles across the shock, it may be explained conceptually in terms of individual particles participating in isolated scattering events.

Consider the trajectories of particles as depicted in Figure 2.6 in the rest frame of a parallel shock, flanked on either side by a turbulent magnetic field convected by a flow that is reducing in speed from upstream to downstream. In this configuration, particles gain energy during head-on collisions with scattering centres in the upstream frame, but lose energy during trailing collisions in the downstream frame. Of course, *collisions* in this context represent pitch-angle¹ scattering mediated by wave-particle interactions. Since the scattering centres in the upstream medium are moving faster than downstream, the net energy change particles experience per scattering cycle is positive. The amount of energy gained per shock crossing depends on the relative energies of the particles and scattering centres, as well as the difference in flow speeds across the shock. See also a similar illustration by *Kallenrode* [1998].

This energy-gain process may also be conceptually explained using diagrams such as shown in Figure 2.7 [see also *Sugiyama et al.*, 2001; *Koskinen*, 2011]. A similar configuration to that shown in Figure 2.6 is assumed, including a parallel shock considered in its rest frame. As an example, the motion of a particle is initially considered relative to the upstream flow speed. Interactions with the local turbulent magnetic field may scatter the particle, but energy is conserved in its local scattering reference frame in which there are no electric fields. The particle therefore

¹The pitch angle refers to the angle between a particle's velocity and the magnetic field. It is formally introduced in Section 3.2.

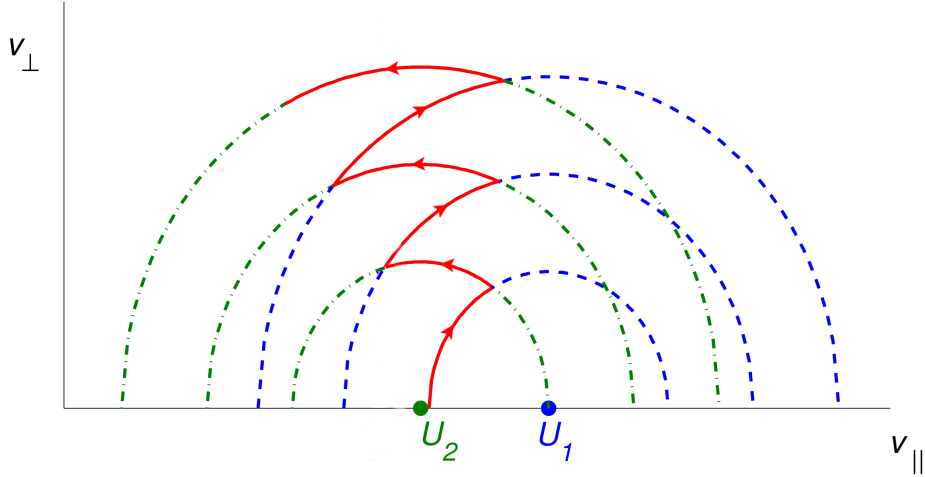


Figure 2.7: An illustration of DSA in velocity space. The blue and green semicircles represent surfaces of constant energy in the reference frames of the upstream and downstream flow speeds, U_1 and U_2 , respectively. Here, $v_{\perp}$ and $v_{\parallel}$ represent particle speed components in the directions perpendicular and parallel to the magnetic field. The red line represents an idealized trajectory of a particle systematically gaining energy by scattering between reference frames. Every intersection of the semicircles along the particle's trajectory represents a scattering event during which the particle crosses the shocks and $v_{\parallel}$ changes signs. Arrows indicate the direction of the particle's movement with time.

remains on constant-energy semicircles in velocity space that are isotropic, *i.e.* centred with respect to the flow speed in the local frame. However, as a result of pitch-angle scattering, energetic particles with velocities greater than the flow speed may travel in either direction relative to the shock (that is, with either $v_{\parallel} < 0$ or $v_{\parallel} > 0$). The particle may therefore cross the shock into the downstream medium, be scattered in that reference frame, and jump to another semicircle centred with respect to the downstream flow speed. In an idealized case, the particle may move to a higher-energy semicircle in the opposite frame with each consecutive shock crossing, thereby gaining energy systematically. See also the related discussion by *Vainio and Afanasiev* [2018].

Note from Figure 2.7 that if the upstream and downstream flow speeds differ by greater amounts, semicircles from different frames would have to be larger to intersect, implying greater energy gains per shock crossing. Should the acceleration process continue until particle speeds (or energies) are much greater than the flow speeds, the vastly enlarged semicircles would appear isotropic (centred) with respect to either frame, implying that prolonged scattering isotropizes velocity (or pitch-angle) distributions. In the present study, DSA is simulated using the *Parker* [1965a] transport equation for isotropic particle distributions as discussed in Chapter 3.

2.4.2 The injection problem

For DSA to be effective, particles must cross the shock front repeatedly. However, particles must be energetic enough in order to return to the shock for repeated shock crossings. Therefore, for particles to participate in the DSA process, their energies (or speeds) must exceed an injection threshold, which refers to the minimum energy E_{inj} , or equivalent particle speed v_{inj} , required to return (or catch up) to the shock. This injection threshold may be estimated in a number of ways [*e.g.* *Neergaard-Parker and Zank*, 2012; *Li et al.*, 2012b; *Hu et al.*, 2017]. However,

the method outlined below is useful to demonstrate some of the dependencies of the injection threshold.

The injection speed may be determined from the requirement that the particle anisotropy Υ must be small at the shock for the DSA formalism to be applicable [Giacalone and Jokipii, 1999; Zank *et al.*, 2006]. As shown by *e.g.* Desai and Giacalone [2016], the anisotropy for the simple case of a parallel shock becomes

$$|\Upsilon|_{\Theta_{BN} \rightarrow 0} \sim \frac{3V_1}{v} \ll 1 \implies v_{\text{inj}} \sim 3V_1, \quad (2.2)$$

which suggest that a particle may be injected into the DSA process if its speed v is larger than the upstream shock-frame flow speed V_1 by a mere factor of 3. Therefore, for parallel or quasi-parallel shocks, where particles can repeatedly cross the shock front along magnetic field lines, injection energies are small. This implies that thermal (Maxwellian-like) distributions may provide sufficiently energetic seed particles for DSA [Giacalone *et al.*, 1992; Neergaard-Parker and Zank, 2012]. The acceleration process at these shocks is enhanced further by the generation of self-excited Alfvénic turbulence [Zank *et al.*, 2006]. In the case of weak scattering at an oblique shock, an altered form of Eq. 2.2 is attained, given by

$$|\Upsilon|_{\kappa_{\parallel} \gg \kappa_{\perp}, \kappa_{r_L}} \sim \frac{3V_1}{v \cos \Theta_{BN}} \ll 1 \implies v_{\text{inj}} \sim \frac{3V_1}{\cos \Theta_{BN}}, \quad (2.3)$$

where $\kappa_{\parallel}$ and $\kappa_{\perp}$ describe diffusion parallel and perpendicular to the magnetic field, while $\kappa_{r_L} = v r_L / 3$, with r_L the gyroradius. The shock obliquity Θ_{BN} is as defined for Eq. 2.1. In this case, injection thresholds for highly oblique shocks are high. Particles only catch up to shock when their speeds exceed $3V_1 / \cos \Theta_{BN}$, which is very fast if $\Theta_{BN} \rightarrow 90^\circ$. Note that $3V_1 / \cos \Theta_{BN}$ is the speed at which the intersection points of magnetic field lines move along the shock front.

Under normal scattering conditions, it is generally true that $\kappa_{\perp} < \kappa_{\parallel}$. This contributes to high rates of acceleration at perpendicular shocks [Giacalone, 2005a, b], owing to more effective confinement of particles at the shock. However, for particles to be accelerated diffusively at highly oblique shocks, they need to be sufficiently energetic already, since their injection thresholds are high [Zank *et al.*, 2006]. These injection energies may be considerably lowered, or become comparable to those of parallel shocks, if field-line meandering is large enough for low-energy particles to experience motion perpendicular to the shock front [Giacalone, 2005a]. This can also be estimated from the limit $\Upsilon \ll 1$ for perpendicular shocks [as shown by Desai and Giacalone, 2016], where

$$|\Upsilon|_{\Theta_{BN} \rightarrow 90^\circ} \sim \frac{3V_1}{v} \sqrt{1 + \left(\frac{\kappa_{r_L}}{\kappa_{\perp}} \right)^2} \ll 1, \quad (2.4)$$

with $\kappa_{\perp} \gg \kappa_{r_L}$, implies that $v_{\text{inj}} \sim 3V_1$, which is the same as for parallel shocks. See also the cases considered by Giacalone and Jokipii [2005], Zank *et al.* [2006], and Li [2017] in the limit where anisotropies are small. Therefore, in the presence of strong magnetic turbulence, either self-generated, such as at parallel shocks, or in the form of field-line meandering at perpendicular shocks, injection thresholds may be lowered so that even thermal particles may be accelerated at shocks [Giacalone, 2005a, b; Zank *et al.*, 2006]. However, in the absence of strong turbulence,

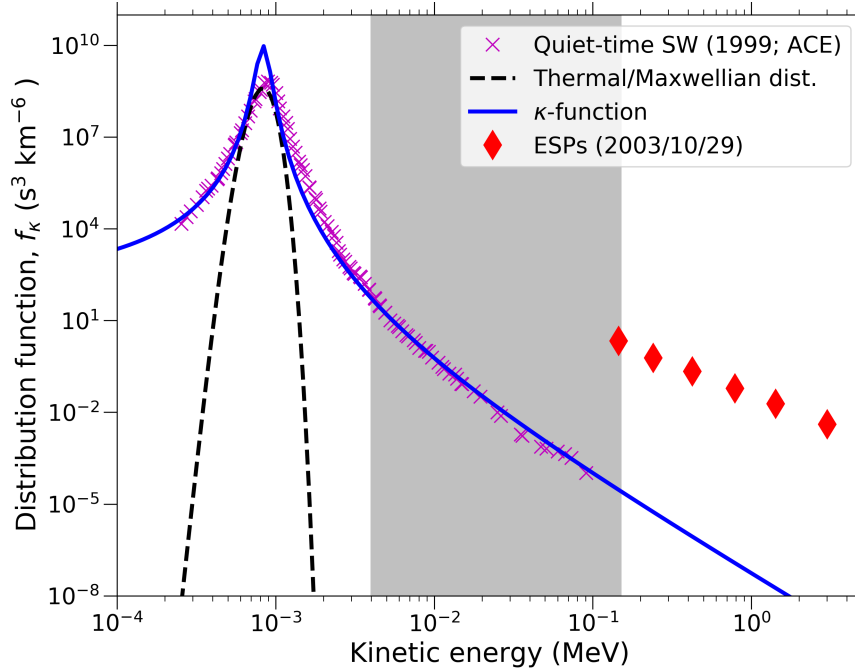


Figure 2.8: Energy distributions of SW particles and ESPs. Observations of the SW distribution (from ACE/ULEIS) in the thermal to suprathermal range for solar-quiet conditions in 1999 are represented by the magenta markers. Observations taken during the Halloween epoch of 2003 (from ACE/EPAM LEMS30/120), shown as an example of ESP enhancements, are represented by the red diamond markers. The dashed black line is a fit of a Maxwellian distribution to the thermal SW distribution, while the blue line represent the κ -function of Eq. 2.5. The shaded region emphasizes the energy range separating the thermal SW distribution from the ESPs.

shock obliquity largely dictates injection thresholds.

Aside from conducive turbulence conditions or shock geometry, injection into the DSA process is also facilitated by the formation of energetic seed particles. In the case of SEPs, this may be achieved by means of prior acceleration in the corona [e.g. *Li et al.*, 2014] or at preceding flares or CME-driven shocks. In fact, reacceleration at successive (or *twin*) CME shocks may accelerate particles up to sufficiently high energies for terrestrial particle detectors to detect them as ground level enhancements [*Li et al.*, 2012a, 2013]. Moreover, injection into the DSA process from the SW is facilitated by the formation of suprathermal tails [*Neergaard-Parker et al.*, 2014; *Zank*, 2017]. The present study considers the heating of the SW distribution during shock passages [see also *Malkov and Voelk*, 1995], which may also increase the number of suprathermal particles capable of exceeding injection thresholds for DSA.

2.5 The suprathermal SW as a source of energetic particles

Suprathermal tails are often observed in SW velocity distributions [*Collier et al.*, 1996; *Maksimovic et al.*, 1997; *Chottoo et al.*, 2000; *Qureshi et al.*, 2003] and are considered to be conducive features for the injection of particles into DSA [*Desai et al.*, 2006; *Kang et al.*, 2014]. Figure 2.8 shows SW observations taken at Earth during solar-quiet conditions. Note that the thermal part of the SW energy distribution can be adequately fitted with a standard Maxwellian distribution, but that distribution cannot account for the suprathermal tail at higher energies.

To describe the SW distribution, *Vasyliunas* [1968] introduces the kappa (κ) distribution function, which is a parameterization that characterizes both the thermal (Maxwellian) core of the SW as well as the suprathermal tail at higher energies. The standard isotropic κ -function is implemented in terms of particle speed v as

$$f_{\kappa} = A_{\kappa} \left(1 + \frac{v^2}{\kappa v_{\kappa}^2} \right)^{-\kappa-1}, \quad (2.5)$$

where v_{κ}^2 is the generalised thermal speed given by

$$v_{\kappa}^2 = (2\kappa - 3) \frac{k_B T}{\kappa m_p}, \quad (2.6)$$

with k_B the Boltzmann constant and m_p the proton mass, and where

$$A_{\kappa} = \frac{n}{(\pi \kappa v_{\kappa}^2)^{3/2}} \frac{\Gamma(\kappa + 1)}{\Gamma(\kappa - \frac{1}{2})} \quad (2.7)$$

is the normalization constant obtained when setting $\int f_{\kappa} d^3v = n$, with n taken as the SW number density and where Γ is the Gamma function. This normalization is discussed in Appendix A. Note that the κ -function fits the SW distribution in Figure 2.8 comparatively well.

The κ -function characterises SW distributions using only three parameters, namely, the κ -parameter, which relates to the spectral index of the suprathermal tail, and the equivalent temperature and number density of the plasma or particle species considered [*Formisano et al.*, 1973; *Chateau and Meyer-Vernet*, 1991]. Note that Eq. 2.5 is defined for $\kappa > 3/2$, and that if $\kappa \rightarrow \infty$, it reduces to a Maxwellian distribution. For the correct interpretation of Eq. 2.6 and the associated temperature T , it is instructive to consider the discussion by *Hellberg et al.* [2009]: v_{κ} is introduced by *Vasyliunas* [1968] as the most probable particle speed, associated with the non-relativistic kinetic energy $E_{\kappa} = m_p v_{\kappa}^2 / 2$. Evaluating the second moment of f_{κ} yields a total energy of $N E_N = \frac{3}{2} N E_{\kappa} \kappa / (\kappa - 3/2)$, where E_N and N are the mean energy per particle and the total number of particles, respectively. Eq. 2.6 then follows upon the introduction of the plasma temperature T [originally by *Formisano et al.*, 1973] through the invocation of the equipartition theorem, $E_N = \frac{3}{2} k_B T$, for a monatomic gas. Although this temperature definition and the foregoing assumption of the equipartition of energy are not strictly valid for non-Maxwellian distributions, their use in this manner has become standard practice [as explained by *Hellberg et al.*, 2009, and the references therein].

It is noted that the κ -distribution can be defined in different ways with respect to how the temperature and thermal speed are defined [*Lazar et al.*, 2016]. Should the temperatures of the κ -distribution and the associated Maxwellian distribution be assumed identical, and a κ -dependent thermal velocity is specified as in Eq. 2.6, the thermal core of the resultant distribution will be enhanced relative to its Maxwellian counterpart. This effect is noticeable from the pronounced core of the distribution shown in Figure 2.8 and implies the presence of some physical process keeping particles at low velocities. By contrast, if (instead of the thermal velocity) the temperature is defined to be κ -dependent, only a high-velocity enhancement occurs, which may be realized in physical terms when collisions between particles are insufficient. Al-

though the latter description likely represents the more frequently realized case in the SW [as discussed by *Lazar et al.*, 2016], either description may be applied in the present study without meaningful differences in their results, because the distributions are similar at large velocities. Furthermore, temperature anisotropies can be calculated from the moments of anisotropic κ -functions [e.g. *Scherer et al.*, 2019], such as the regularized κ -functions introduced by *Scherer et al.* [2017]. However, for the purposes of the present study, the standard κ -function is applied to describe the SW distribution. Note that this study does not address how the κ -distributed suprathermal tails are formed, nor does it posit that DSA at interplanetary shocks is necessarily responsible for their formation. For reviews on the theory and applications of κ -functions, see e.g. *Pierrard and Lazar* [2010] and *Livadiotis and McComas* [2013].

Note that quantities such as the plasma density and temperature are observed to change during the passage of an interplanetary shock [e.g. *Lario and Decker*, 2002], which also transforms the κ -function. As mentioned in the closing paragraph of Section 2.4, the present study considers the heating of the SW distribution, in response to the evolution of the aforementioned plasma quantities during shock passages, as a mechanism for energizing potential seed particles for DSA. Given the large separation between typical ESP energies and the thermal SW, as illustrated in Figure 2.8, injecting particles from a heated SW distribution may facilitate the reproduction of typical ESP intensities. This is explored further in Chapter 4.

2.6 Summary

This chapter introduces the necessary background for the present study, including brief discussions regarding the SW, the heliospheric magnetic field, and the formation of CMEs and CIRs. The typical properties for travelling shocks in the inner heliosphere are also reviewed. In particular, shocks associated with CMEs and CIRs are considered. These shocks are typically fast-mode shocks that can accelerate energetic particles.

Moreover, DSA is discussed as a mechanism for accelerating energetic particles at shocks. Important factors impacting on the efficiency of this mechanism are reviewed. These include the relative geometries of the shock and the local magnetic field, or shock obliquity, as well as the importance of turbulence in both the injection of particles into the DSA process and their confinement near the shock. Given that the DSA formalism is applicable where particle anisotropies are small, its effects are simulated in subsequent chapters using the *Parker* [1965a] equation for near-isotropic distributions.

The SW distribution is considered as a source population for energetic particles in this study. To characterize the SW velocity distribution, the κ -function is implemented. As a central theme of the present study, the evolution of the SW distribution in response to shock-induced changes in plasma parameters is investigated. The aims of this are twofold. Firstly, the heating of the SW distribution by shocks serves to energize potential seed particles for DSA, and secondly, these heated SW particles may aid in reproducing particle intensity enhancements at typical ESP energies by injecting more seed particles at higher energies.

Chapter 3

Modelling particle transport and acceleration using stochastic differential equations

3.1 Introduction

This chapter introduces the theoretical and modelling concepts required to simulate the shock acceleration process within the broader context of energetic particle transport. DSA at shocks throughout the inner heliosphere relies on reasonably strong scattering conditions, which tend to isotropize particle distributions. Section 3.2 introduces a distribution function representing near-isotropic particle distributions and relates it to other commonly used measures of particle abundances. The modulation of the distribution function, subject to various particle transport and energy-change processes (including DSA), is discussed in Section 3.3. This section also introduces the relevant TPE, which is solved in various forms depending on the complexity of the applications considered.

The latter part of the chapter elaborates on the numerical methods applied to solve the TPE. Section 3.4 discusses the derivation and application of stochastic differential equations (SDEs) that provide solutions that are equivalent to those of Fokker-Planck-type TPEs. These SDEs are solved for the majority of the applications in this study using a time-backward approach, owing to its efficiency. The equivalent time-forward approach is used for the sake of illustration in Section 3.5 to provide an introduction to modelling DSA. Finally, an importance sampling technique is introduced in Section 3.5.2 to increase the efficiency of the time-forward SDE method.

3.2 Counting particles

This section introduces the omni-directional distribution function to represent particle abundances, and discusses how it relates to more familiar quantities such as the particle number density and differential intensity. The latter is commonly used to present particle abundances

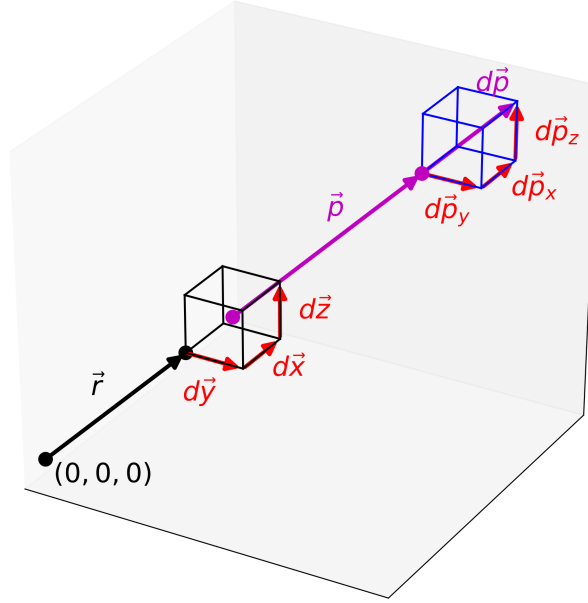


Figure 3.1: Representations of volumes in configuration and momentum space, d^3x and d^3p , for which the distribution function is defined according to Eq. 3.1. d^3x contains all the particles at position $\vec{r}$ with a momentum $\vec{p}$ in d^3p .

from spacecraft observations. Differential intensity is therefore also the preferred format for presenting results in this study. See also *Moraal* [2013] for more on these quantities.

3.2.1 The distribution function and number density

Consider a number of particles $d\mathcal{N}$ in a small volume d^3x at a position $\vec{r} = (x, y, z)$ and with momentum in d^3p around $\vec{p} = (p_x, p_y, p_z)$ as illustrated in Figure 3.1. The distribution function $f(\vec{r}, \vec{p}, t)$ is introduced such that

$$d\mathcal{N} = f(\vec{r}, \vec{p}, t) d^3x d^3p. \quad (3.1)$$

This can be related to the ordinary number density n by integrating over all momentum space,

$$n = \int f(\vec{r}, \vec{p}, t) d^3p. \quad (3.2)$$

The above volume integral can be re-written by considering a momentum coordinate system as shown in Figure 3.2. Assuming the gyro-centre at the origin and the magnetic field line about which the particle gyrates to be along p_z , that is $\vec{B} = B\hat{e}_z$, the azimuthal angle ϕ_p represents the particle's gyrophase and the polar angle θ_p its pitch angle.

This allows the momentum-space volume element to be expressed in spherical coordinates as $d^3p = p^2 d\Omega dp$, where $d\Omega = \sin\theta_p d\theta_p d\phi_p$ is a solid-angle element about $\vec{p}$, and $p = |\vec{p}|$ is the particle's scalar momentum. Noting that $\vec{p}$ can hence be expressed in terms of the coordinates (p, ϕ_p, θ_p) , Eq. 3.2 can be rewritten as

$$n = \int_0^\infty \int_0^{2\pi} \int_0^\pi p^2 f(\vec{r}, p, \theta_p, \phi_p, t) \sin\theta_p d\theta_p d\phi_p dp = \int_0^\infty p^2 \int_\Omega f(\vec{r}, p, \theta_p, \phi_p, t) d\Omega dp, \quad (3.3)$$

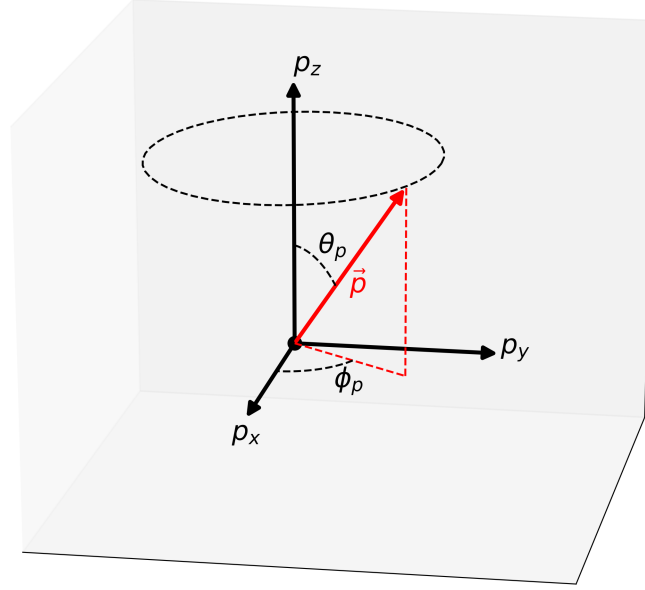


Figure 3.2: A spherical momentum coordinate system, where p_z is along the magnetic field line and the particle momentum $\vec{p}$ is defined in terms of the scalar momentum p , gyro-phase angle ϕ_p and pitch angle θ_p .

where $\int_{\Omega}$ represents the integral over all solid angles. However, since particle detectors typically cannot resolve statistically significant numbers of particles incident from only one particular direction, the average number of particles per unit solid angle in momentum space is considered. Accordingly, the omni-directional distribution function (that is, averaged over all directions in $\vec{p}$ -space for a fixed p) is defined as

$$f_0(\vec{r}, p, t) = \frac{\int_{\Omega} f(\vec{r}, \vec{p}, t) d\Omega}{\int_{\Omega} d\Omega} = \frac{1}{4\pi} \int_{\Omega} f(\vec{r}, \vec{p}, t) d\Omega, \quad (3.4)$$

since $\int_{\Omega} d\Omega = \int_0^{2\pi} d\phi_p \int_0^{\pi} \sin \theta_p d\theta_p = 4\pi$. Note that $f_0(\vec{r}, p, t)$ is the distribution function solved for in the *Parker* [1965a] transport equation discussed in Section 3.3. Note further from Eq. 3.4 that $f(\vec{r}, \vec{p}, t)$ can be taken out of the integral over solid angle if it is assumed to be isotropic, that is, independent of both ϕ_p and θ_p . In this case it follows that $f(\vec{r}, \vec{p}, t) \approx f_0(\vec{r}, p, t)$. From Eqs. 3.3 and 3.4 the number density can be expressed as

$$n = \int_0^{\infty} 4\pi p^2 f_0(\vec{r}, p, t) dp \quad (3.5)$$

$$= \int_0^{\infty} U_p(\vec{r}, p, t) dp, \quad (3.6)$$

where $U_p(\vec{r}, p, t) = 4\pi p^2 f_0(\vec{r}, p, t)$ is known as the differential number density. Here, U_p represents the number density between two spherical shells in $\vec{p}$ -space with radii of p and $p + dp$, respectively. While spacecraft cannot resolve volume densities, U_p does prove to be useful to relate the quantities they measure to those introduced above [Gleeson and Axford, 1967; Gleeson and Urch, 1973].

3.2.2 Toward the differential intensity

Spacecraft essentially measure the flux of particles observed for a particular viewing direction within a particular momentum (or energy) band. This is known as the differential intensity j_p , and is the number of particles detected per momentum interval per unit time per unit area of observed space per unit solid angle. Dimensionally, this can be attained by the product of the differential number density and the speed at which particles move toward the detector through a surface perpendicular to their motion, averaged over all solid angles. That is,

$$j_p(\vec{r}, p, t) = \frac{v U_p(\vec{r}, p, t)}{4\pi} = v p^2 f_0(\vec{r}, p, t), \quad (3.7)$$

which, in turn, relates the differential intensity to the distribution function. It is useful to express the differential intensity in terms of kinetic energy to compare with spacecraft observations. The conversion of j_p , expressed per momentum interval dp , to j_E , expressed per interval of kinetic energy dE , is carried out by noting that $j_p dp = j_E dE$ due to the conservation of particles. It hence follows that

$$j_E = j_p \frac{dp}{dE}. \quad (3.8)$$

Note that since $p^2 = (E_T^2 - E_0^2) / c^2$, where $E_T = E + E_0$ with E_T , E and E_0 denoting the total, kinetic, and rest-mass energies, respectively, it follows that

$$\frac{dp}{dE} = \frac{E + E_0}{pc^2} = \frac{E_T}{pc^2} = \frac{\gamma m_0 c^2}{\gamma m_0 v c^2} = \frac{1}{v}, \quad (3.9)$$

where γ is the Lorentz factor and m_0 is the rest mass. Then, using Eq. 3.8, j_E can be related to the distribution function as

$$j_E = \frac{j_p(\vec{r}, p, t)}{v} = p^2 f_0(\vec{r}, p, t), \quad (3.10)$$

which, in this study, is given in units of particles $\text{m}^{-2} \text{s}^{-1} \text{sr}^{-1} \text{MeV}^{-1}$.

3.3 Modelling the transport of energetic particles

The present study is primarily concerned with particle acceleration by travelling interplanetary shocks. It is assumed that the propagation times of these shocks are large compared to the pitch-angle scattering time, or equivalently that particles undergo many scattering events in the time that elapses during shock passages. Such strong scattering conditions serve to isotropize pitch-angle distributions, which allow the distribution function to be approximated by the omni-directional (or pitch angle averaged) distribution function introduced in Eq. 3.4. The modulation of energetic particles represented by an omni-directional distribution function $f = f_0(\vec{r}, p, t)$ can be described by the *Parker* [1965a] TPE,

$$\frac{\partial f}{\partial t'} = \nabla \cdot (\mathbf{K} \cdot \nabla f) - \vec{V}_{sw} \cdot \nabla f + \frac{1}{3} (\nabla \cdot \vec{V}_{sw}) \frac{\partial f}{\partial \ln p} + Q, \quad (3.11)$$

in terms of time, position, and scalar momentum. The terms, from left to right, describe time-dependent changes, spatial diffusion, convection with the SW, energy changes as a result of transport in regions of expanding or compressing SW flows, and a source term Q , with the quantities $\mathbf{K}$ and $\vec{V}_{sw}$ being the diffusion tensor and the SW velocity respectively. Since Eq. 3.11 is valid for near-isotropic particle distributions associated with strong scattering, it describes particle transport in the diffusive limit. This is adequate to describe DSA and particle transport around the time of shock passages [as also motivated by *Giaccalone, 2015*], but renders it less suitable for the description of energetic particle events (or phases thereof) that are associated with large particle anisotropies and characterized by streaming-limited transport and weak scattering [*Reames and Ng, 1998*].

Furthermore, while omitted in Eq. 3.11, the *Parker* [1965a] TPE can be derived to include a second-order momentum diffusion term. This can be used to simulate stochastic acceleration by the interaction of particles with the electromagnetic fields produced by flux rope dynamics, which may also modify the effects of DSA [*le Roux et al., 2015, 2016*]. It is noted that the aforementioned acceleration may also serve as a mechanism for energizing seed particles for DSA at interplanetary shocks. However, the present study particularly aims to investigate the heating of the SW distribution as a mechanism to energize particles for injection into DSA. With this in mind, and to avoid concealing the effects of DSA, the momentum diffusion term is omitted.

3.3.1 SW velocity and velocity divergence

In order to obtain steady-state solutions for $\partial f / \partial t' = 0$, and apply a time-stationary magnetic field expression, the TPE is solved in a frame rotating with the Sun [*Kota and Jokipii, 1983*]. The SW velocity in this frame is given by

$$\vec{V}_{sw} = \vec{V}'_{sw} - \vec{\Omega} \times \vec{r} = V'_{sw} \hat{e}_r - \Omega_{\odot} r \sin \theta \hat{e}_{\phi}, \quad (3.12)$$

where the SW velocity is assumed to be spherically symmetric in the frame that is not rotating with the Sun, that is, $\vec{V}'_{sw} = V'_{sw} \hat{e}_r$, and where $\vec{\Omega}$ is the Sun's rotation vector with an angular speed of $\Omega_{\odot} = 2.67 \times 10^{-6} \text{ rad s}^{-1}$. From Eq. 3.12 it follows that the divergence only has a radial component, that is

$$\nabla \cdot \vec{V}_{sw} = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 V'_{sw}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (-\Omega_{\odot} r \sin \theta) = \frac{2V'_{sw}}{r} + \frac{\partial V'_{sw}}{\partial r}. \quad (3.13)$$

The first term on the right-hand side of the equation above is positive, representing regions of expanding SW flow, which, in the corresponding term in the TPE, results in particles experiencing adiabatic energy losses. Given the $1/r$ -dependence, these energy losses tend to be more prevalent in the inner heliosphere. The second term becomes relevant in regions of compressed SW flow, such as shocks, where it is negative, resulting in energy gains in the corresponding TPE term. The effects of DSA are therefore implicitly simulated in the TPE for particles being scattered across the aforementioned regions. This is also subject to certain matching conditions across the shock [*Steenberg and Moraal, 1999*]. However, it is explained in Section 3.4 that their explicit specification is not necessary when solving the TPE using the SDE approach. Note fur-

thermore that since particle intensities are presented more often in terms of kinetic energy than momentum, the term in the TPE governing energy changes is rewritten as

$$\frac{1}{3} (\nabla \cdot \vec{V}_{sw}) \frac{\partial f}{\partial \ln p} \equiv \frac{1}{3r^2} \frac{\partial}{\partial r} (r^2 V'_{sw}) \left(\frac{E + 2E_p}{E + E_p} \right) E \frac{\partial f}{\partial E}, \quad (3.14)$$

where the momentum is related to the kinetic energy according to $p = (1/c)\sqrt{E(E + 2E_p)}$ for protons with E_p the proton rest-mass energy.

3.3.2 A 3D spherical diffusion tensor

Particle scattering is governed by coefficients describing the diffusion of particles relative to magnetic field lines. The diffusion tensor associated with a field-aligned coordinate system, with an axis parallel to the average magnetic field, similar to that shown in Figure 3.2, and the other axes perpendicular to it, is given by

$$\mathbf{K}_B = \begin{bmatrix} \kappa_{||} & 0 & 0 \\ 0 & \kappa_{\perp\theta} & 0 \\ 0 & 0 & \kappa_{\perp r} \end{bmatrix}, \quad (3.15)$$

where $\kappa_{||}$ is the diffusion coefficient describing diffusion parallel to the magnetic field, and $\kappa_{\perp\theta}$ and $\kappa_{\perp r}$ describe diffusion perpendicular to the magnetic field. Note that to consider magnetic field curvature, gradient, and current sheet drifts, drift coefficients may be included in the tensor above. However, as is shown in later chapters, shock-accelerated spectra terminate at energies typically smaller than 10 MeV for the applications considered in this study. At these low energies, drifts are significantly reduced in the presence of turbulence, and are therefore not expected to affect these shock-accelerated particles significantly [see also *Engelbrecht and Burger, 2015; Engelbrecht et al., 2017*]. The descriptions of the coefficients $\kappa_{||}$, $\kappa_{\perp\theta}$, and $\kappa_{\perp r}$ are given as appropriate for the applications considered in each of the subsequent chapters.

The TPE is solved in spherical coordinates, which requires the diffusion tensor of Eq. 3.15 to be transformed accordingly. Figure 3.3 depicts a 3D magnetic field geometry. Following *e.g. Burger et al. [2008]*, two angles are defined, namely

$$\zeta = \tan^{-1} \left(\frac{B_\theta}{B_r} \right), \quad (3.16)$$

which is the angle between the projection of the magnetic field onto the (r, θ) -plane and the radial direction, and

$$\psi = \tan^{-1} \left(\frac{-B_\phi}{\sqrt{B_r^2 + B_\theta^2}} \right), \quad (3.17)$$

which is the angle between the magnetic field itself and the projection of the field onto the (r, θ) -plane. Here, B_r , B_ϕ , and B_θ represent the radial, azimuthal, and polar components of the magnetic field, which, expressed in terms of its magnitude B , ζ , and ψ , is given by

$$\vec{B} = B \cos \psi \cos \zeta \hat{e}_r + B \cos \psi \sin \zeta \hat{e}_\theta - B \sin \psi \hat{e}_\phi, \quad (3.18)$$

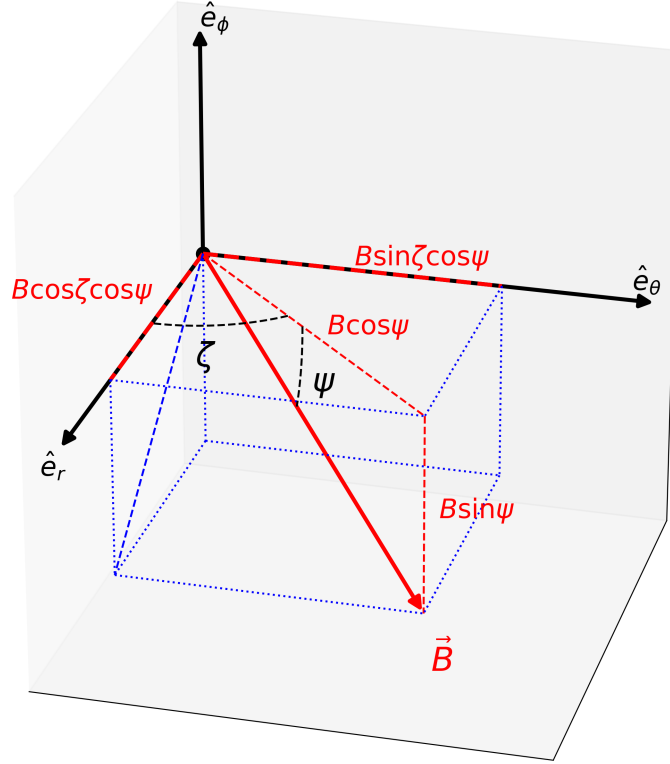


Figure 3.3: Decomposition of a 3D magnetic field in terms of the angles ζ and ψ , as defined for Eqs 3.16 and 3.17, respectively. The dashed red lines represent components of the magnetic field in each of the spherical coordinates, as well as the projection of the field onto the (r, θ) -plane. The dashed blue line is a projection of the field onto the (r, ϕ) -plane, which is equivalent to the *Parker* [1958] field if $B_\theta = 0$.

as can be inferred from Figure 3.3. To construct a transformation matrix to transform Eq. 3.15 from field-aligned to spherical coordinates, base vectors are constructed for the former set of coordinates. They are determined from

$$d\vec{B} = \frac{\partial \vec{B}}{\partial B} dB + \frac{\partial \vec{B}}{\partial \zeta} d\zeta + \frac{\partial \vec{B}}{\partial \psi} d\psi = \vec{g}_1 dB + \vec{g}_2 d\zeta + \vec{g}_3 d\psi \quad (3.19)$$

to be

$$\begin{aligned} \vec{e}_1 &= \frac{\vec{g}_1}{|\vec{g}_1|} = \cos \psi \cos \zeta \hat{e}_r + \cos \psi \sin \zeta \hat{e}_\theta - \sin \psi \hat{e}_\phi \\ \vec{e}_2 &= \frac{\vec{g}_2}{|\vec{g}_2|} = -\sin \zeta \hat{e}_r + \cos \zeta \hat{e}_\theta \\ \vec{e}_3 &= -\frac{\vec{g}_3}{|\vec{g}_3|} = \sin \psi \cos \zeta \hat{e}_r + \sin \psi \sin \zeta \hat{e}_\theta + \cos \psi \hat{e}_\phi, \end{aligned} \quad (3.20)$$

where $\vec{e}_3 = \vec{e}_1 \times \vec{e}_2$ for right-handed coordinate system. The transformation matrix hence follows as

$$\mathbf{T}^{-1} = \begin{bmatrix} \cos \psi \cos \zeta & \cos \psi \sin \zeta & -\sin \psi \\ -\sin \zeta & \cos \zeta & 0 \\ \sin \psi \cos \zeta & \sin \psi \sin \zeta & \cos \psi \end{bmatrix}, \quad (3.21)$$

from which the diffusion tensor for a 3D magnetic field is written in spherical coordinates as

$$\mathbf{K} = \mathbf{T}\mathbf{K}_B\mathbf{T}^{-1} = \begin{bmatrix} \kappa_{rr} & \kappa_{r\theta} & \kappa_{r\phi} \\ \kappa_{\theta r} & \kappa_{\theta\theta} & \kappa_{\theta\phi} \\ \kappa_{\phi r} & \kappa_{\phi\theta} & \kappa_{\phi\phi} \end{bmatrix},$$

with elements given by

$$\begin{aligned} \kappa_{rr} &= \kappa_{\perp\theta} \sin^2 \zeta + \cos^2 \zeta (\kappa_{\parallel} \cos^2 \psi + \kappa_{\perp r} \sin^2 \psi) \\ \kappa_{\theta r} &= \kappa_{r\theta} = \sin \zeta \cos \zeta (\kappa_{\parallel} \cos^2 \psi + \kappa_{\perp r} \sin^2 \psi - \kappa_{\perp\theta}) \\ \kappa_{\theta\phi} &= \kappa_{\phi\theta} = (\kappa_{\perp r} - \kappa_{\parallel}) \sin \psi \cos \psi \sin \zeta \\ \kappa_{\phi r} &= \kappa_{r\phi} = (\kappa_{\perp r} - \kappa_{\parallel}) \sin \psi \cos \psi \cos \zeta \\ \kappa_{\phi\phi} &= \kappa_{\parallel} \sin^2 \psi + \kappa_{\perp r} \cos^2 \psi \\ \kappa_{\theta\theta} &= \kappa_{\perp\theta} \cos^2 \zeta + \sin^2 \zeta (\kappa_{\parallel} \cos^2 \psi + \kappa_{\perp r} \sin^2 \psi). \end{aligned} \quad (3.22)$$

Note from Figure 3.3 that if $B_\theta = 0$ it implies that $\zeta = 0$, in which case ψ becomes the angle between the average magnetic field and the radial direction, and the standard *Parker* [1958] magnetic field is retrieved. In this case, the diffusion tensor simplifies accordingly, as shown in Section 5.2. Note also that the definitions of ζ and ψ given in Eqs 3.16 and 3.17, and the resultant transformation matrix, are not unique [see *e.g.* *Kobylinski*, 2001; *Alania*, 2002]. See also the generalized diffusion tensor by *Effenberger et al.* [2012], which accounts for anisotropic perpendicular diffusion.

Incorporating Eqs 3.12, 3.14, and 3.22 into the TPE, its most general form applied in this study is written in three spatial dimensions and spherical coordinates as

$$\begin{aligned} \frac{\partial f}{\partial t'} &= \left(\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \kappa_{rr}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\kappa_{\theta r} \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial \kappa_{\phi r}}{\partial \phi} - V'_{sw} \right) \frac{\partial f}{\partial r} \\ &+ \left(\frac{1}{r^2} \frac{\partial}{\partial r} (r \kappa_{r\theta}) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (\kappa_{\theta\theta} \sin \theta) + \frac{1}{r^2 \sin \theta} \frac{\partial \kappa_{\phi\theta}}{\partial \phi} \right) \frac{\partial f}{\partial \theta} \\ &+ \left(\frac{1}{r^2 \sin \theta} \frac{\partial}{\partial r} (r \kappa_{r\phi}) + \frac{1}{r^2 \sin \theta} \frac{\partial \kappa_{\theta\phi}}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial \kappa_{\phi\phi}}{\partial \phi} + \Omega_\odot \right) \frac{\partial f}{\partial \phi} \\ &+ \frac{2\kappa_{r\phi}}{r \sin \theta} \frac{\partial^2 f}{\partial r \partial \phi} + \frac{2\kappa_{r\theta}}{r} \frac{\partial^2 f}{\partial r \partial \theta} + \frac{2\kappa_{\theta\phi}}{r^2 \sin \theta} \frac{\partial^2 f}{\partial \theta \partial \phi} \\ &+ \kappa_{rr} \frac{\partial^2 f}{\partial r^2} + \frac{\kappa_{\theta\theta}}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \frac{\kappa_{\phi\phi}}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2} \\ &+ \frac{1}{3r^2} \frac{d}{dr} (r^2 V'_{sw}) \xi(E) E \frac{\partial f}{\partial E} + Q, \end{aligned} \quad (3.23)$$

where $\xi(E) = (E + 2E_p)/(E + E_p)$. This TPE is simplified as appropriate for each application considered in the following chapters. Chapter 4 considers a spherically symmetrical configuration in which the TPE is solved for a single spatial dimension. Chapters 5 and 6 consider multidimensional applications. In particular, the TPE in the form of Eq. 3.23 is solved in Chapter 6 to simulate acceleration at compression waves associated with CIRs.

3.4 Formulating the stochastic differential equations

The TPE specified in multiple computational dimensions typically requires numerical methods to solve. The transport and DSA of energetic particles are simulated here by solving an equivalent set of SDEs [see also *Kruells and Achterberg, 1994; Marcowith and Kirk, 1999; Zhang, 2000*]. The advantages and limitations of this method are discussed in Section 3.4.2. The aspects of the SDE approach that are important for this study are detailed below. Refer to *Strauss and Effenberger [2017]* for a comprehensive review.

The derivation of SDEs equivalent to the TPE depends on whether they are to be solved in a time-forward or time-backward fashion. These approaches are equivalent, but the time-backward approach is generally more efficient. In this approach, an observational point $\vec{x}_{\text{obs}}$ is chosen that represents the combination of coordinates at which the value of the distribution function is sought at a particular time. Solving the SDEs yields trajectories of phase-space density elements, or *pseudo particles*, in terms of each of the coordinates. These pseudo particles are traced backwards in time until they sample a particle source region (*e.g.* a shock), where they are assigned a weight according to the value of the source function Q in the TPE. This process is explained further in Section 3.4.1. A time-backward parameter t is defined in terms of the usual time(-forward) parameter t' according to

$$t = t_T - t', \quad (3.24)$$

where t_T represents the total time of the simulation. For a time-backward simulation, the integration of the SDEs is performed for $t = 0 \rightarrow t_T$. In Chapters 4 and 5, t_T is defined as the duration of a CME shock's transit to Earth, whereas in Chapter 6 it is associated with the time required to rotate through a particular angle at the rate of solar rotation. Note that $\partial/\partial t' = -\partial/\partial t$, since t_T is assumed to be constant.

The general formulation for a n_d -dimensional set of SDEs is given in the form of the Itô equation [see also *Zhang, 1999*] as

$$dx_i = \mu_i(x_i, t) dt + \sum_{j=1}^{n_d} \sigma_{ij}(x_i, t) dW_j(t), \quad (3.25)$$

with $\vec{x} = (r, \phi, \theta, E)$ and where $dW_i = \Lambda_i(t)\sqrt{dt}$ represents the multidimensional Wiener process for Gaussian-distributed pseudo-random numbers $\Lambda_i(t)$, the vector $\vec{\mu}$ represents an n_d -dimensional vector containing convective transport coefficients corresponding to each coordinate in $\vec{x}$, and σ is a $n_d \times n_d$ matrix similarly containing diffusive transport coefficients. The SDEs may be inferred from the TPE cast into the form of the time-backward Kolmogorov equation, given by

$$-\frac{\partial f(x_i, t)}{\partial t} = \sum_{i=1}^{n_d} \mu_i(x_i, t) \frac{\partial f(x_i, t)}{\partial x_i} + \frac{1}{2} \sum_{i=1}^{n_d} \sum_{j=1}^{n_d} D_{ij}(x_i, t) \frac{\partial^2 f(x_i, t)}{\partial x_i \partial x_j}, \quad (3.26)$$

where $D_{ij}(x_i, t) = \sigma_{ij}(x_i, t) \cdot \sigma_{ij}(x_i, t)^T$, with $\sigma_{ij}(x_i, t)$ as defined for Eq. 3.25. The SDEs equiv-

alent to the TPE of Eq. 3.23 may therefore be written in the form of the Itô equation for each coordinate as

$$\begin{aligned} dr &= \mu_r dt + \sigma_{rr} dW_r + \sigma_{r\theta} dW_\theta + \sigma_{r\phi} dW_\phi \\ d\theta &= \mu_\theta dt + \sigma_{\theta\theta} dW_\theta + \sigma_{\theta\phi} dW_\phi \\ d\phi &= \mu_\phi dt + \sigma_{\phi\phi} dW_\phi \\ dE &= \mu_E dt, \end{aligned} \quad (3.27)$$

with

$$\begin{aligned} \mu_r &= \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \kappa_{rr}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\kappa_{r\theta} \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial \kappa_{\phi r}}{\partial \phi} - V'_{sw} \\ \mu_\theta &= \frac{1}{r^2} \frac{\partial}{\partial r} (r \kappa_{r\theta}) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (\kappa_{\theta\theta} \sin \theta) + \frac{1}{r^2 \sin \theta} \frac{\partial \kappa_{\phi\theta}}{\partial \phi} \\ \mu_\phi &= \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial r} (r \kappa_{r\phi}) + \frac{1}{r^2 \sin \theta} \frac{\partial \kappa_{\theta\phi}}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial \kappa_{\phi\phi}}{\partial \phi} + \Omega_\odot \\ \mu_E &= \frac{1}{3r^2} \frac{\partial}{\partial r} (r^2 V'_{sw}) E \xi(E), \end{aligned} \quad (3.28)$$

and where

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{rr} & \sigma_{r\theta} & \sigma_{r\phi} \\ \sigma_{\theta r} & \sigma_{\theta\theta} & \sigma_{\theta\phi} \\ \sigma_{\phi r} & \sigma_{\phi\theta} & \sigma_{\phi\phi} \end{bmatrix}, \quad (3.29)$$

is a triangular matrix with elements [also used by *Pei et al.*, 2010] given by

$$\begin{aligned} \sigma_{rr} &= \sqrt{\frac{2 \left(\kappa_{\phi\phi} \kappa_{r\theta}^2 - 2 \kappa_{r\phi} \kappa_{r\theta} \kappa_{\theta\phi} + \kappa_{rr} \kappa_{\theta\phi}^2 + \kappa_{\theta\theta} \kappa_{r\phi}^2 - \kappa_{rr} \kappa_{\theta\theta} \kappa_{\phi\phi} \right)}{\kappa_{\theta\phi}^2 - \kappa_{\theta\theta} \kappa_{\phi\phi}}} \\ \sigma_{r\theta} &= \frac{\kappa_{r\phi} \kappa_{\theta\phi} - \kappa_{r\theta} \kappa_{\phi\phi}}{\kappa_{\theta\phi}^2 - \kappa_{\theta\theta} \kappa_{\phi\phi}} \sqrt{2 \left(\kappa_{\theta\theta} - \frac{\kappa_{\theta\phi}^2}{\kappa_{\phi\phi}} \right)} \\ \sigma_{r\phi} &= \frac{\sqrt{2} \kappa_{r\phi}}{\sqrt{\kappa_{\phi\phi}}} \\ \sigma_{\theta\theta} &= \frac{1}{r} \sqrt{2 \left(\kappa_{\theta\theta} - \frac{\kappa_{\theta\phi}^2}{\kappa_{\phi\phi}} \right)} \\ \sigma_{\theta\phi} &= \frac{\sqrt{2} \kappa_{\theta\phi}}{r \sqrt{\kappa_{\phi\phi}}} \\ \sigma_{\phi\phi} &= \frac{\sqrt{2} \kappa_{\phi\phi}}{r \sin \theta}, \end{aligned} \quad (3.30)$$

with $\sigma_{\theta r} = \sigma_{\phi r} = \sigma_{\phi\theta} = 0$. Note that $\boldsymbol{\sigma}$ as given here is not uniquely determined, but is merely one possibility of a set of mathematically equivalent matrices that satisfy $D_{ij}(x_i, t) = \sigma_{ij}(x_i, t) \cdot \sigma_{ij}(x_i, t)^T$ [e.g. *Johnson et al.*, 2002].

Starting from the observational point, the SDEs in Eq. 3.27 are solved iteratively using the Euler-Maruyama numerical scheme [*Maruyama*, 1955] for a finite time step Δt . The Euler-Maruyama scheme has a first-order weak convergence. Higher-order numerical schemes may

be derived from the truncated stochastic Taylor expansions of each coordinate's SDE in integral form. Examples of such schemes include the Milstein scheme, which yields comparable results to the Euler-Maruyama scheme when solving the *Parker* [1965a] TPE [e.g. *Wawrzynczak et al.*, 2015]. These schemes often involve higher-order derivatives of coefficients. In cases where these derivatives are very complicated, the application of Runge-Kutta-type numerical schemes may be more appropriate, since in those schemes derivatives are calculated numerically. Given that the coefficients of the SDEs considered for the applications in this study tend to be either constant or slowly varying, the application of the Euler-Maruyama scheme is sufficient. See also *Kloeden and Platen* [1995] for an overview on higher-order numerical SDE schemes.

Note that when solving the SDEs the time is not incremented by the same amount during each iteration. It is instead specified to vary, depending on the dominant radial transport process at the current position, to maintain a fixed step length that is related to the shock thickness. The time step is therefore specified according to [*Strauss and Effenberger*, 2017]

$$\Delta t = \min \left\{ \frac{0.1L}{|\mu_r|}, \frac{0.1L^2}{\max(|\sigma_{rr}|, |\sigma_{r\theta}|, |\sigma_{r\phi}|)} \right\}. \quad (3.31)$$

This has at least two advantages: firstly, limiting the step length to some fraction of the length scale L , which is associated with the shock, ensures that the shock structure is properly sampled. Only processes acting in the radial direction are included in the calculation of this variable time step, because, as per Eq. 3.14, particle heating at the shock results only because of the change in the SW speed in the radial direction. Secondly, scaling Δt in this manner saves computation time, since instead of applying a very small fixed time step, Δt will only be small when it is required. As a result of this variable time step, computation times are typically longer for larger values of the transport coefficients, such as the diffusion coefficients at higher energies, and for narrower shocks with smaller associated L -values.

3.4.1 Handling the source function and DSA in the SDE approach

When modelling DSA in the TPE using finite-difference methods, it is also necessary to specify matching conditions across the shock [*Steenberg and Moraal*, 1999]. These conditions ensure the continuity of the distribution function across the shock, and that the particle flux diverging from the shock should have its source on the shock. For the SDE approach, these conditions are satisfied implicitly.

It is instructive to consider pseudo particles in terms of the mathematical realizations of the distribution function they represent. Pseudo-particle trajectories connect all points in coordinate space along which the distribution function remains constant, or stated differently, they represent paths along which Liouville's theorem holds. Therefore, should a pseudo particle be traced back from the observational point $\vec{x}_{\text{obs}}$ to a point $\vec{x}_*$ coinciding with the shock at some earlier time t^* , it follows that $f(\vec{x}_{\text{obs}}) = f(\vec{x}_*)$. Also, because only pseudo particles that have interacted with the shock are of interest for DSA, some fraction of the value of the source function (Q in the TPE), specified at the shock, is attributed to $f(\vec{x}_{\text{obs}})$. These pseudo-particle trajectories are therefore implicitly compliant with the matching conditions referred to earlier.

The source function Q in the TPE is handled in the SDE approach as a correction term [Strauss and Effenberger, 2017]. Expressing it as a rate of contribution to the distribution function allows the contribution per pseudo particle (or its *amplitude*) to be calculated iteratively along the integration trajectory. That is, $Q = d\alpha/dt \implies \Delta\alpha = Q\Delta t$, from which it follows that

$$\alpha_i(t - \Delta t) = \alpha_i(t) + Q\Delta t, \quad (3.32)$$

with $\alpha_i(t = 0) = 0$. The source contribution is then tallied for N_p pseudo particles such that

$$f_{\text{obs}}(\vec{x}_{\text{obs}}) = \frac{1}{N_p} \sum_{i=1}^{N_p} \alpha_i \quad (3.33)$$

gives the value of the distribution function at the observational point at the time $t' = t_T$ (or $t = 0$). Section 4.2.2 introduces the source function and discusses its specification. Furthermore, physical particle distributions can also be obtained by tallying the amplitude-weighted flux contributions of pseudo particles within appropriately sectorized spatial and energy intervals (or *bins*) at any time during the simulation, divided by the number of pseudo particles counted within each sector. This method is used in *e.g.* Section 4.6.3 to trace likely acceleration sites and seed-particle energies in a time-backward fashion. A similar binning technique is also utilized in a time-forward fashion in Section 3.5.

3.4.2 Advantages and limitations of the SDE approach

The SDE approach has been successfully applied in many instances to simulate space particle transport [Zhang, 1999; Pei *et al.*, 2010; Strauss *et al.*, 2011, 2013; Moloto *et al.*, 2019] and DSA in particular [Kruells and Achterberg, 1994; Marcowith and Kirk, 1999; Zhang, 2000; Zuo *et al.*, 2011; Hu *et al.*, 2017]. The time-backward approach is favoured here due to its efficiency, since every simulated pseudo particle contributes to intensities at the desired observational point. Additionally, in a similar fashion to how the boundary interactions of pseudo particles are used to trace the most probable points of entry into the heliosphere for cosmic rays [*e.g.* Strauss *et al.*, 2013], this backward tracing of phase-space trajectories is similarly utilized in this study to map probable acceleration sites and seed-particle energies. This technique is used in Sections 4.6, 5.5, and 6.7. Since these pseudo-particle trajectories are solved entirely independent of each other, this approach is also conducive to the utilization of parallel computing platforms.

However, this mutual independence of the SDE solutions also limits applications to the test-particle case. Non-linear effects of shock acceleration such as self-generated turbulence [Lee, 1983; le Roux and Arthur, 2017] or particle mediation of shock structures [Mostafavi *et al.*, 2017] can therefore not be considered. Moreover, any process that requires the calculation of particle intensity gradients becomes computationally expensive [*e.g.* Moloto *et al.*, 2019]. Nevertheless, the SDE approach remains suitable to investigate the intricacies of classical DSA, without the limitations imposed by a numerical grid, such as instabilities involving multiple computational dimensions and the large gradients that are typically encountered at shocks. It is shown in Appendix B.1 that the SDEs produce appreciably similar results to a finite-difference approach

in reproducing ESP events for the same parameter set.

Furthermore, as opposed to finite-differences schemes, the SDE model introduced in this study can seamlessly be expanded to a larger number of computational dimensions [e.g. *Pei et al.*, 2010] as required to study particle acceleration at more complicated shock geometries. This is demonstrated in Chapters 4 through 6, as more computational dimensions are required to model applications of increasing complexity.

3.5 A proof-of-concept model for shock acceleration

This section introduces a proof-of-concept model for the purpose of demonstrating the features of DSA in the context of a simple hypothetical transport configuration that is not necessarily physically representative. The applications considered in following chapters make use of the time-backward SDE approach, owing to its efficiency compared to the time-forward method. Given the emphasis of the time-backward approach elsewhere, a time-forward SDE model is employed in this section for illustrative purposes.

For the purposes of this proof-of-concept SDE model for DSA, a simplified form of the TPE in Eq. 3.11 is considered for a single spatial dimension in Cartesian coordinates,

$$\frac{\partial f}{\partial t'} = -V_x \frac{\partial f}{\partial x} + \frac{\partial}{\partial x} \left(\kappa_x \frac{\partial f}{\partial x} \right) + \frac{p}{3} \frac{dV_x}{dx} \frac{\partial f}{\partial p}, \quad (3.34)$$

where $V_x = V_x(x)$ and κ_{xx} are the one-dimensional flow speed and diffusion coefficient, respectively. Note that particles are not added as a source, but are handled as an initial condition. At the start of the simulation, pseudo particles are thus released at the shock ($x_0 = 0$) with an initial momentum corresponding to a rigidity of ~ 2 GV ($p_0 \approx 10^{-18}$ kg m s $^{-1}$). To obtain the equivalent time-forward SDEs, this simplified TPE must be written in the form of the time-forward Kolmogorov equation, given by

$$\frac{\partial f(x_i, t')}{\partial t'} = - \sum_{i=1}^{n_d} \frac{\partial}{\partial x_i} (\mu_i(x_i, t') f(x_i, t')) + \frac{1}{2} \sum_{i=1}^{n_d} \sum_{j=1}^{n_d} \frac{\partial^2}{\partial x_i \partial x_j} (D_{ij}(x_i, t') f(x_i, t')), \quad (3.35)$$

where the coefficients are as previously defined for Eqs 3.25 and 3.26. This implies that Eq. 3.34 needs to be rewritten in conservative form, as

$$\frac{\partial F}{\partial t'} = - \frac{\partial}{\partial x} \left(\left(\frac{\partial \kappa_{xx}}{\partial x} + V_x \right) F \right) + \frac{\partial^2}{\partial x^2} (\kappa_{xx} F) + \frac{\partial}{\partial p} \left(\frac{p}{3} \frac{dV_x}{dx} F \right), \quad (3.36)$$

where the transformation $F = p^2 f$ is applied. For simplicity, κ_{xx} is assumed to be a constant. The SDEs in the form of the Itô equation for spatial position and momentum then follow as

$$\begin{aligned} dx &= V_x dt' + \sqrt{2\kappa_{xx} dt'} \Lambda(t') \\ dp &= -\frac{p}{3} \frac{dV_x}{dx} dt', \end{aligned} \quad (3.37)$$

The spatial SDE above is the equivalent of a diffusion-convection equation, while the other

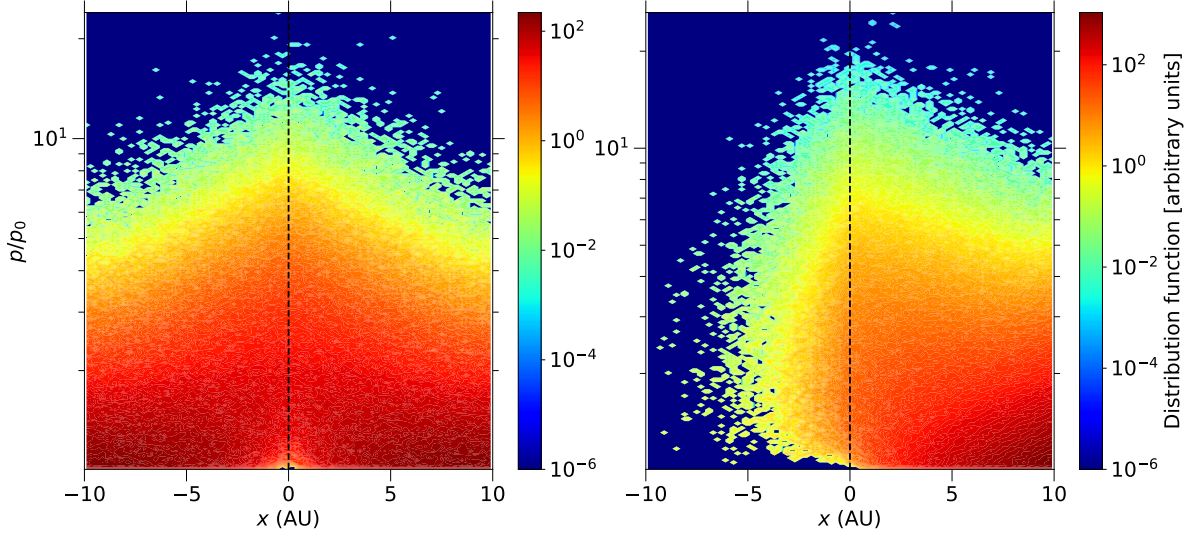


Figure 3.4: Spatial (x) and momentum (p) distributions of pseudo particles for diffusive transport across the shock, with and without the effects of convection as shown in the right and left panels, respectively. Note that the momentum scale is expressed as multiples of the initial momentum p_0 . The vertical dashed line indicates the shock position at $x = 0$.

describes the incremental momentum change owing to the particle's interaction with the shock. Note that in this case the SDEs are solved for a fixed time step of $\Delta t = 374$ seconds and a total simulation time of $t_T = 25000 \Delta t$, repeated for a million pseudo particles.

3.5.1 A first look at features of DSA

The trajectories of pseudo particles are solved from Eq. 3.37, subject to the simple transport configuration described below. The flow speed is specified to transition across a stationary shock at $x = 0$ according to

$$V_x = \frac{V_x^0}{2s} \left((s+1) - (s-1) \tanh\left(\frac{x}{L}\right) \right), \quad (3.38)$$

such that

$$\frac{dV_x}{dx} = \frac{V_x^0}{2sL} (1-s) \cosh^{-2}\left(\frac{x}{L}\right), \quad (3.39)$$

where V_x^0 is the flow speed value at $x/L \ll 0$, s is the compression ratio, and L is related to the ramp width of the shock transition. The reference values of the flow speed and diffusion coefficient are chosen to be $V_x^0 = 400 \text{ km s}^{-1}$ and $\kappa_{xx}^0 = 6 \times 10^{20} \text{ cm}^2 \text{ s}^{-1}$, respectively. The compression ratio is chosen as $s = 2$, and $L = 0.5 \text{ AU}$, unless specified otherwise. Reflective spatial boundaries are specified at $x_{\min} = -10 \text{ AU}$ and $x_{\max} = 10 \text{ AU}$, such that $x = 2x_{\min} - x$ if $x < x_{\min}$, and $x = 2x_{\max} - x$ if $x > x_{\max}$. The number of particles is binned in terms of position and momentum at selected instances in time, which according to Eq. 3.1 provides a representation of the distribution function.

Examples of these distributions are shown in Figure 3.4, which illustrates the effects of diffusion, both with and without the effects of convection as shown in the right and left panels, respectively. Where the effects of convection are neglected, only the convection term in the

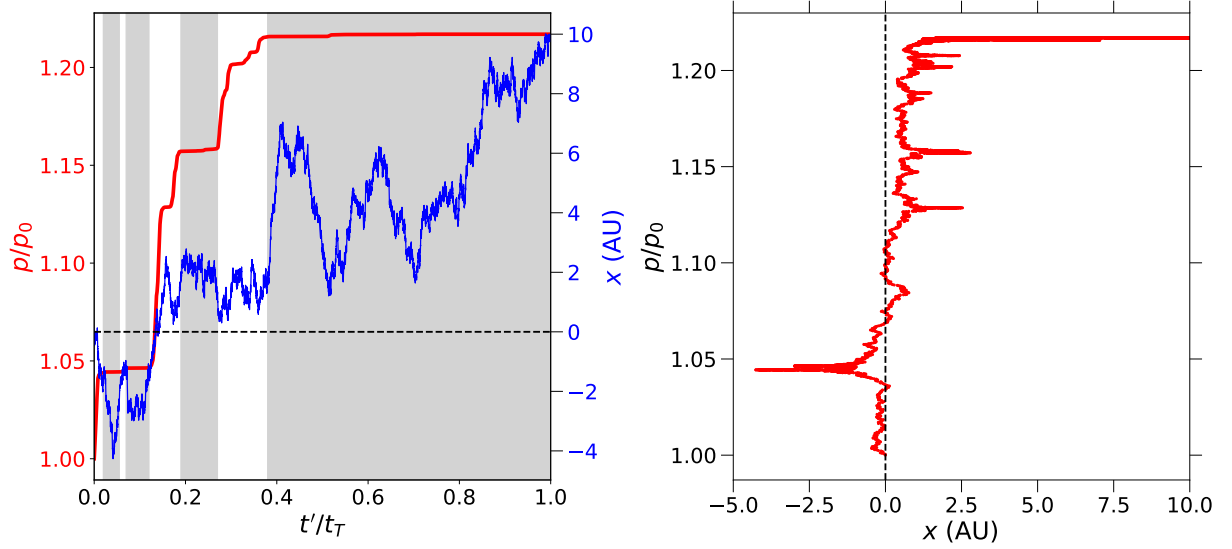


Figure 3.5: Left: Sample trajectories of a pseudo particle in x and p -space, as shown in blue and red, respectively, as functions of time. The time is expressed as a fraction of the total simulation time of $t_T = 25000 \Delta t$, with $\Delta t = 374$ s. The shaded regions indicate selected periods during which the particle shows negligible change in momentum, corresponding to periods during which the particle is far from the shock, which is indicated at $x = 0$ with a dashed horizontal line. Right: Plot of momentum against position for the pseudo particle trajectories shown on the left. Note that the momentum plateaus when the particle does not interact with the shock region.

TPE is set to zero. Note that in either case, particle momenta extend to higher values in the vicinity of the shock, at $x = 0$, owing to their acceleration at that position. In terms of their distribution around the shock, diffusion tends to arrange particles symmetrically, resembling the Gaussian distribution according to which the pseudo-random numbers in the Wiener process are distributed. The right panel of Figure 3.4 shows the effect of including convection in the positive x -direction, which predictably skews the distribution of particles toward that direction. It is instructive to consider the spatial and momentum trajectories of a single pseudo particle as shown in the left panel of Figure 3.5. Note that the particle only gains momentum when it moves either across or near to the shock (indicated by white regions on the figure), where the momentum gain for the latter case follows from the fact that the shock has a finite width related to L . By contrast, when the particle moves further away from the shock, the momentum remains unchanged (as indicated by the grey shaded areas). This is also demonstrated by the plot in the right panel of Figure 3.5, where momentum values similarly plateau for either $x \ll 0$ or $x \gg 0$, but increase when $x \approx 0$. Repeated transport in the compressed flow speed regions near the shock therefore facilitates the acceleration of particles to larger momenta. Particles may diffuse across the shock repeatedly, especially under strong scattering conditions simulated by small κ_{xx} -values.

To explore how the acceleration of particles diffusing across the shock may be affected by changing conditions, the parameters s , κ_{xx} , and L are varied with the effects of convection neglected. In this case, the spatial SDE in Eq. 3.37 is equivalent to a simple diffusion equation. The left and right panels of Figure 3.6 show the momentum distributions of particles accelerated at the shock for varying diffusion coefficients and ramp widths, respectively. Decreasing the value of the diffusion coefficient extends distributions to larger momenta. Smaller diffusion

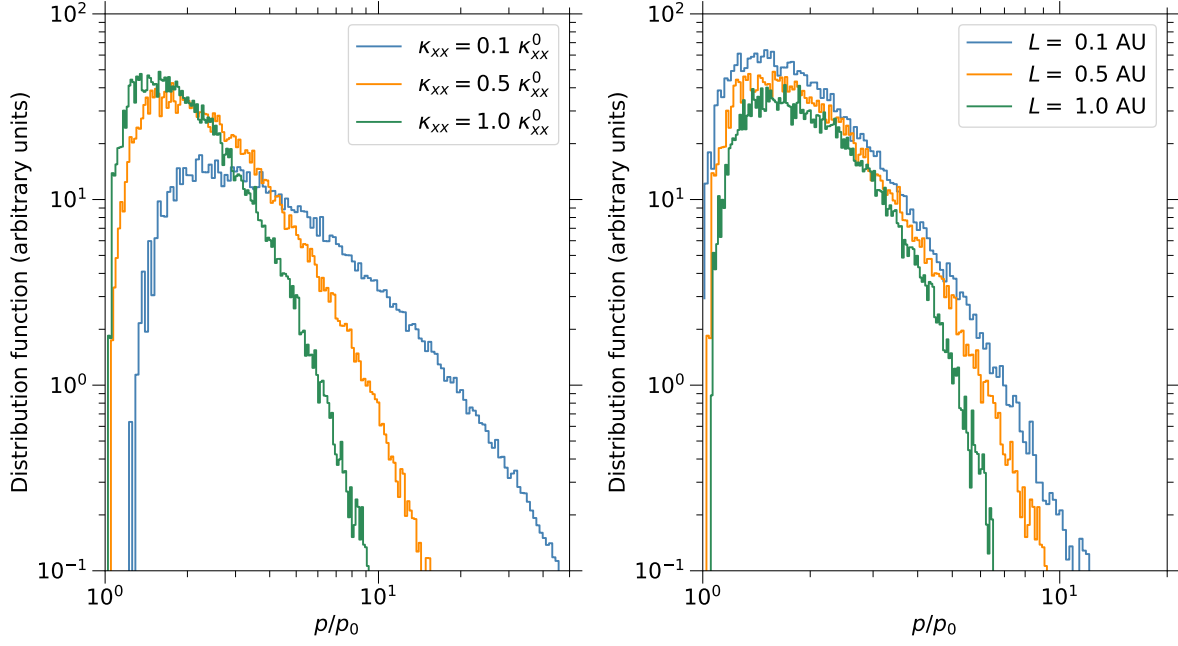


Figure 3.6: Momentum distributions at the shock's position at $x = 0$ for varying values of the diffusion coefficient and shock width, as shown in the left and right panels, respectively.

coefficients implies stronger scattering, which serves to confine particles near the shock. This allows more time for particles to be accelerated, resulting in their distributions extending to larger momenta. In the right panel of Figure 3.6, smaller shock ramp widths similarly result in distributions extending to larger momenta. This follows because the rate of momentum gain, *i.e.* $dp/dt' = -(p/3)(dV_x/dx) \sim -(p/3)(V_x/L)$, is larger for smaller L -values, which allows distributions to extend to larger momenta within the available time frame.

The left panel of Figure 3.7 shows the time evolution of momentum distributions at the shock. Note that pseudo particles are not continually injected into the system, but released at the shock with an initial momentum p_0 only at the start of the simulation ($t' = 0$). Therefore, it follows from the conservation of the number of particles that the areas under the curves at different instances in time remain the same. Distributions extend to larger momenta at the expense of their values at smaller momenta. Note furthermore that at least a segment of the momentum distribution is aligned with the power law p^{-4} at all stages of its evolution. As time progresses, these segments move toward larger momenta as the distribution is accelerated further. The maximum attainable momentum is therefore shown to be time-limited. Distribution functions with this form of momentum dependence are a quintessential feature of DSA. The right panel of Figure 3.7 shows that the power-law index changes for varying compression ratios. These indices correspond to the values predicted by DSA according to

$$\gamma_f = -\frac{3s}{s-1}, \quad (3.40)$$

where s is the compression ratio, as previously defined, and γ_f represents the momentum power-law index of a shock-accelerated distribution function, $f \propto p^{\gamma_f}$. The equivalent power-law index for DSA-produced energy spectra (converted to differential intensity by means of Eq. 3.10) is introduced in Section 4.4.

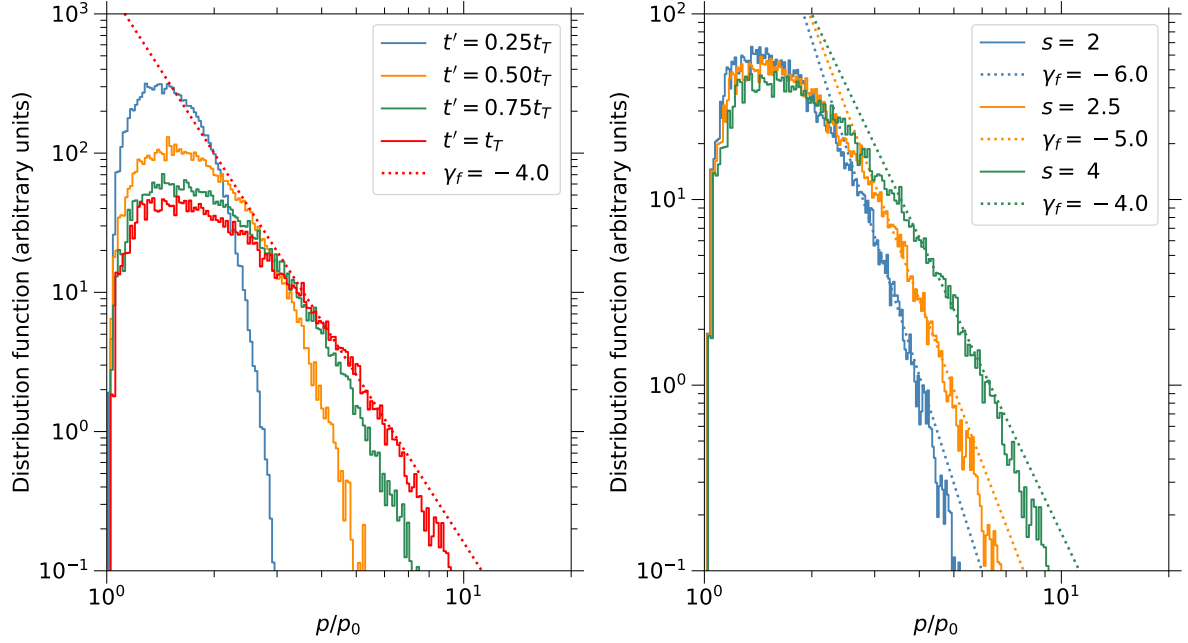


Figure 3.7: Left: Time evolution of momentum distributions at the shock's position. The total simulation time is given by $t_T = 25000 \Delta t$, with $\Delta t = 374$ s. Right: Momentum distributions for varying compression ratios. Dotted lines represent power laws with indices as given by Eq. 3.40 and indicated in the figure legend.

The simulated momentum distributions display several features of classical DSA, despite the simplicity of the transport configuration applied in this section. Many of these features, including those relating to the relative sizes of the diffusion coefficients and shock widths, the time progression and compression ratio, are revisited in Chapter 4 for a more realistic application.

3.5.2 Modelling DSA with importance sampling

It has already been mentioned that the time-forward SDE approach is less efficient than the time-backward approach because not all pseudo particles may necessarily sample regions of interest. For example, in the context of DSA, if too few pseudo particles sample the shock during the simulation, or if they do not spend sufficient time near the shock, momentum distributions may terminate prematurely, because pseudo particles have insufficient time to be accelerated up to higher momenta in significantly large numbers. Stated differently, higher momenta may be statistically underrepresented as a result of poor numerical shock sampling. Whereas these statistics may be improved by simulating a greater number of pseudo particle trajectories, computationally, this becomes exponentially more expensive. Instead, an importance sampling technique may be implemented as discussed below. See also the similar discussion by *Strauss and Effenberger* [2017].

Pseudo particles may be forced to spend more time in the vicinity of the shock (and thereby be further accelerated) by means of including an artificial convection term in the TPE. However, this must be implemented in such a manner that it improves numerical sampling without introducing physical transport effects. To do this, the distribution function is transformed as

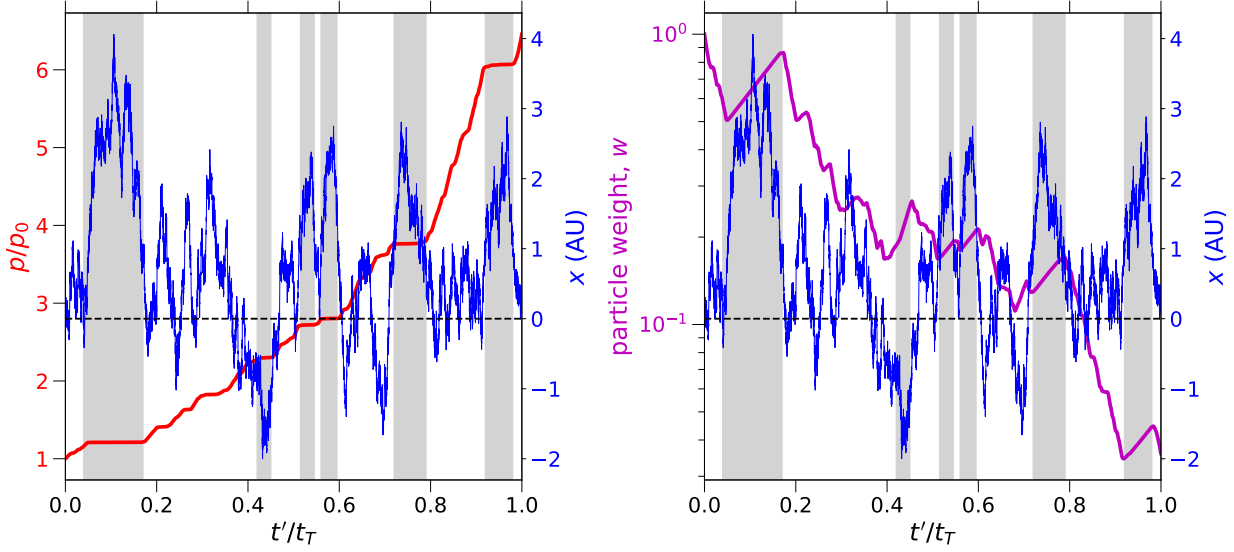


Figure 3.8: Left: Similar to the left panel of Figure 3.5, but with the effects of importance sampling included. Right: Similar to the trajectories shown on the left, but showing the time evolution of the particle weight, as described by Eq. 3.51, instead of the momentum. As in Figure 3.5, shaded regions indicate selected periods during which the particle moves far away from the shock.

follows

$$f(x, p, t') = A(x) h(x, p, t'), \quad (3.41)$$

where $A = A(x)$ is a function only of the spatial coordinate x and $h = h(x, p, t')$ is the transformed distribution function. Note that all boundary and initial conditions must similarly be transformed for the setup to remain consistent. The specification of A is discussed further below. Eq. 3.34 then becomes

$$\frac{\partial h}{\partial t'} = -\frac{V_x}{A} \frac{\partial A h}{\partial x} + \frac{1}{A} \frac{\partial}{\partial x} \left(\kappa_{xx} \frac{\partial A h}{\partial x} \right) + \frac{p}{3} \frac{dV_x}{dx} \frac{\partial h}{\partial p}. \quad (3.42)$$

To infer the equivalent SDE formulation, the above TPE must be rewritten (as discussed in Appendix B.2) in the form of Eq. 3.35 as

$$\frac{\partial H}{\partial t'} = -\frac{\partial}{\partial x} \left(\left(\frac{\partial \kappa_{xx}}{\partial x} + V_x - \frac{2\kappa_{xx}}{A} \frac{dA}{dx} \right) H \right) + \frac{\partial^2}{\partial x^2} (\kappa_{xx} H) + \frac{\partial}{\partial p} \left(\frac{p}{3} \frac{dV_x}{dx} H \right) + \mathcal{L}H, \quad (3.43)$$

where $H = p^2 h$. In this form, the TPE gains an additional linear term $\mathcal{L}H$ with a coefficient of

$$\mathcal{L} = - \left(\frac{\partial \kappa_{xx}}{\partial x} + V_x - \frac{2\kappa_{xx}}{A} \frac{dA}{dx} \right) \frac{1}{A} \frac{dA}{dx} - \frac{\kappa_{xx}}{A} \frac{d^2 A}{dx^2}. \quad (3.44)$$

The SDEs for x and p can be readily inferred from Eq. 3.43 as

$$dx = \left(V - \frac{2\kappa_{xx}}{A} \frac{dA}{dx} \right) dt' + \sqrt{2\kappa_{xx} dt'} \Lambda(t'), \quad (3.45)$$

$$dp = -\frac{p}{3} \frac{dV}{dx} dt', \quad (3.46)$$

where κ_{xx} is again assumed to be a constant, and all symbols are as previously defined.

Comparing the SDEs and associated TPE for the case without importance sampling (Eqs 3.36 and 3.37) to those above, two differences are noted. The first is the artificial convection term, which depends on a virtual flow speed given by $-2\kappa_{xx}(dA/dx)/A$. For the present application, this term is chosen in a manner that would facilitate the transport of pseudo particles toward the shock. To this end, A is specified as

$$A(x) = \left(\cosh \left(\frac{x}{L} \right) \right)^{A_0 L}, \quad (3.47)$$

so that

$$\frac{1}{A} \frac{dA}{dx} = A_0 \tanh \left(\frac{x}{L} \right), \quad (3.48)$$

and

$$\frac{1}{A} \frac{d^2 A}{dx^2} = \left(\frac{1}{A} \frac{dA}{dx} \right)^2 + \frac{A_0}{L} \left(1 - \tanh^2 \left(\frac{x}{L} \right) \right), \quad (3.49)$$

where A_0 is a scaling constant. Larger values of A_0 imply stronger artificial convection. In the case where $A_0 \rightarrow 0$, all derivatives of A reduce to zero and $A \rightarrow 1$, which would imply that $f(x, p, t') = h(x, p, t')$ such as for a case where importance sampling is not applied. Note from the expression for $(dA/dx)/A$ that the artificial convection term in Eq. 3.45 acts in the same direction as V_x for $x < 0$, but acts in the opposite direction of V_x for $x > 0$. In either case, it serves to transport particles toward the shock at $x = 0$. This artificially prolongs the residency of particles near the shock, which improves acceleration efficiency. This is demonstrated in the left panel of Figure 3.8, where it is shown that the particle returns to the shock more frequently under the influence of the artificial convection described by Eq. 3.48. As a result, the particle also gains momentum more frequently and ultimately attains a larger momentum value at the end of the simulation.

The second difference when including importance sampling is the appearance of the linear term $\mathcal{L}H$. It is noted that $\mathcal{L}H$ should have dimensions consistent with those of the transformed distribution function H per unit time, and can therefore be expressed in terms of a rate as

$$\frac{dw}{dt'} = \mathcal{L}w \implies w = w_0 e^{\mathcal{L}t'}, \quad (3.50)$$

where w is introduced as the *particle weight*. Note that $w_0 = 1$ is the particle weight at the start of the simulation. This particle weight is solved simultaneously with Eqs 3.45 and 3.46 for each pseudo particle according to

$$w_i(t' + \Delta t') = w_i(t') e^{\mathcal{L}\Delta t}, \quad (3.51)$$

in a time-forward fashion for a fixed time step of $\Delta t = 374$ s. Normally, pseudo particles would invariably be assigned a weight of unity. However, owing to the presence of the linear term $\mathcal{L}H$ in the TPE, the particle weight varies to compensate for the artificially prolonged time spent near the shock. As illustrated in the right panel of Figure 3.8, in the presence of the artificial convection toward the shock, the weight of the pseudo particle decreases when moving toward the shock and increases when moving away.

When constructing H using a binning procedure, the contributions of each pseudo particle must be weighted according to its w -value, instead of simply tallying the number of particles

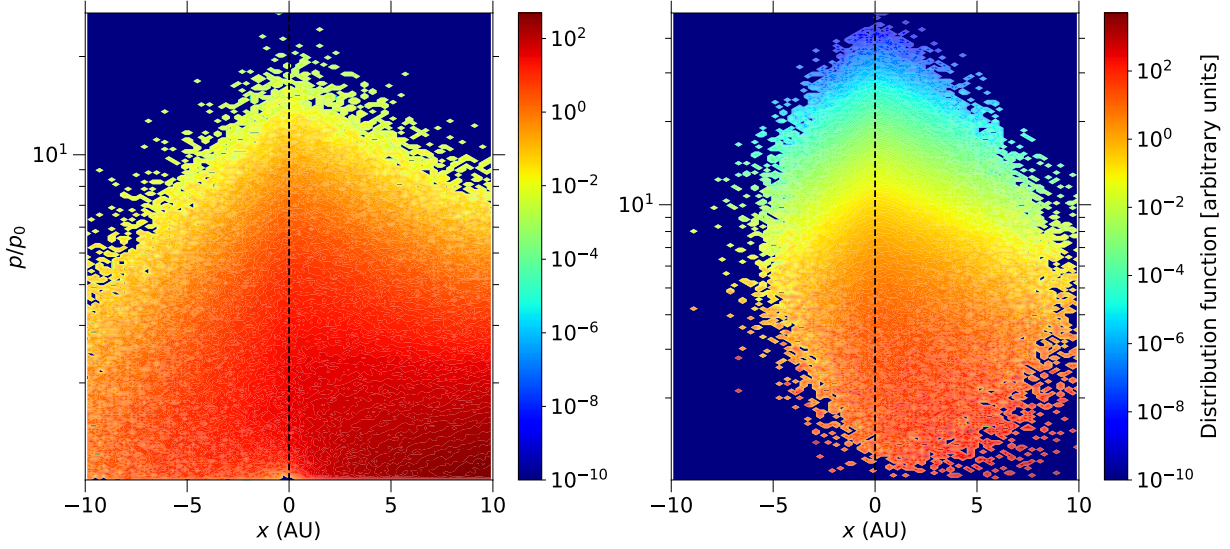


Figure 3.9: Similar to Figure 3.4, but with $V_x = 0.5V_x^0$, and for cases with and without the effects of importance sampling, as shown in the right and left panels, respectively. The strength of the artificial convection toward the shock, as described by Eq. 3.48, is scaled with $A_0 = 0$ and 0.5 for the cases shown in the left and right panels, respectively.

within each (x, p) -bin. The transformations of Eq. 3.41 and $H = p^2 h$ are applied in reverse to retrieve the distribution function represented by $f(x, p, t')$. The effects of importance sampling on $f(x, p, t')$ are presented in Figures 3.9 and 3.10. Comparing the distributions with and without importance sampling in Figure 3.9, the effects of this technique are evident. Firstly, this technique indeed favours the transport of pseudo particles toward the shock, which improves the shock sampling rate. This comes at the obvious expense of sampling in regions further removed from the shock. However, given the emphasis on shock acceleration, these regions are of lesser interest. As a result of the artificial convection toward the shock, particles gain momentum more frequently, and adequate statistical representation is achieved at larger momenta. Note that the maximum momentum attained when including importance sampling where $A_0 = 0.5$ is $p/p_0 \sim 50$, compared to $p/p_0 \sim 20$ for $A_0 = 0$. Even though the momentum distribution attains a maximum momentum that is at best only a factor of ~ 2.5 larger when including importance sampling, the range of the distribution function is increased by roughly 8 orders of magnitude across the extended momentum domain.

The importance sampling does not, however, alter the qualitative properties of the shock-accelerated momentum distributions. This is demonstrated in Figure 3.10, which shows that for larger A_0 -values, the momentum distribution indeed extends to larger momenta, but also that the distribution function in this extended momentum domain conforms to the predicted DSA form. It does not, for example, extend the power-law segment, but merely improves particle statistics in the exponentially decreasing phase. The effects of importance sampling are therefore entirely numerical, improving the efficiency of the time-forward SDE approach when modelling DSA, but without changing the physics of the acceleration process.

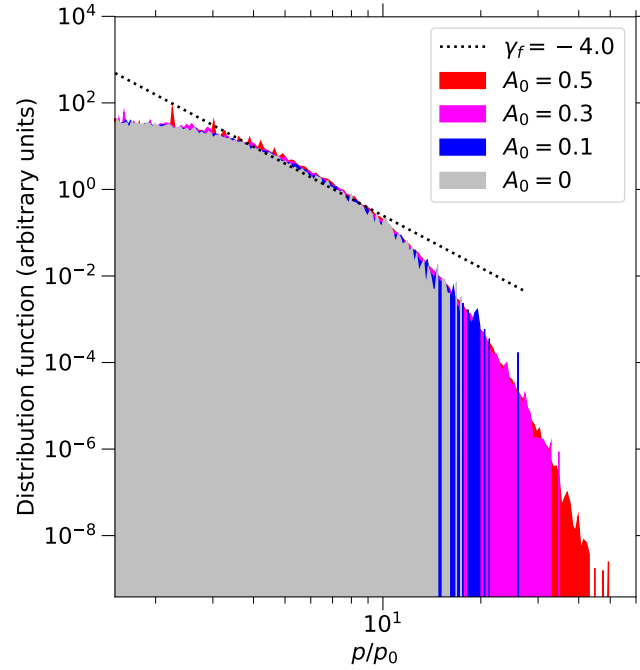


Figure 3.10: Momentum distributions including the effects of importance sampling for various values of A_0 , scaling the strength of the artificial convection described by Eq. 3.48. The dotted line represents a power law with an index given by Eq. 3.40 for a compression ratio of $s = 2$.

3.6 Summary and conclusions

This chapter introduces a general description of energetic particle transport. The *Parker* [1965a] TPE is introduced to describe the modulation of near-isotropic distributions of energetic particles. These particles are subject to various transport and energy-change processes. In particular, the SW velocity is defined for a frame rotating with the Sun, whereas the effects of DSA are incorporated into an adiabatic energy-change term involving the SW velocity divergence. In compressed regions in the SW, such as shocks, particles gain energy by means of scattering between magnetic irregularities in the converging SW flow. The effects of DSA are simulated using this mechanism. The scattering process is represented in the TPE by means of coefficients describing particle diffusion relative to magnetic field lines. These diffusion coefficients are transformed to spherical coordinates and arranged in a tensor describing particle diffusion relative to a 3D magnetic field. Section 3.3 hence presents a TPE that describes changes in the distribution function relative to three spatial dimensions, energy, and time. In subsequent chapters, this TPE is simplified and its transport coefficients specified as appropriate for each of the applications considered.

The TPE is solved in this study by means of solving an equivalent set of SDEs as derived in Section 3.4. This approach is chosen owing to its numerical stability and flexibility, especially with respect to its seamless expansion to larger numbers of computational dimensions. It does however limit applications to the test-particle case. Moreover, a time-backward approach is implemented. This entails tracing the trajectories of pseudo particles backwards in time from the point in parameter space where the value of the distribution function is sought (also known as the observational point) in each coordinate. Since every pseudo particle contributes to the

distribution function at the observational point, this approach is computationally efficient. Furthermore, given the continuity of the distribution function along pseudo-particle trajectories, the SDE approach also implicitly complies with the matching conditions for DSA across the shock.

As a separate application, an introduction to the features of DSA is given in Section 3.5 for a simple transport configuration. For this application, the time-forward SDE approach is employed, which entails releasing pseudo particles at a stationary shock, and binning their positions and momenta at some later time during the simulation. The properties of momentum distributions are shown to depend on various parameters related to the shock. It is shown, as theoretically expected, that DSA arranges momentum distributions according to power laws depending on the shock compression ratio. The power-law distributions are shown to extend to larger momenta for smaller diffusion coefficients, since stronger scattering implies that particles are confined near the shock for longer, allowing more time for acceleration. The same result is attained by extending the simulation time. It is also shown that broader shocks result in less efficient acceleration, since the rate of momentum gain is smaller. These concepts recur in the present study, and are revisited in Chapter 4 in particular.

Although the time-forward approach is relatively inefficient when solving the TPE for particular points in parameter space, Section 3.5.2 demonstrates how this approach may be improved by means of applying an importance sampling technique. This technique involves a transformation of the distribution function, where the transformation factor is chosen such that an artificial convection term appears in the TPE that serves to transport particles toward the shock. As a result of the increased time particles spend near the shock, aiding their acceleration, a greater number of particles attain larger momenta. The statistics of particle distributions at these large momenta are therefore significantly improved. The contributions of particles toward the distribution function are also scaled according to a weight compensating for the artificially prolonged time the particles may spend near to the shock. It is demonstrated that this importance sampling technique is useful to improve particle statistics at points in the parameter space that are of interest, without altering physical characteristics.

Note that subsequent chapters draw on the transport and numerical configurations introduced in Sections 3.3 and 3.4. Also, for all of the following applications, the TPE is solved using the time-backward SDE approach, which is adequately efficient without applying importance sampling.

Chapter 4

Acceleration of solar wind particles at travelling shocks

4.1 Introduction

Energetic particle enhancements observed at Earth are often associated with the passage of interplanetary shocks, driven by CMEs during ESP events. These enhancements are thought to occur as a result of particle acceleration at the shock, for which DSA is regarded a viable mechanism, often coupled with self-generated turbulence in the form of magnetohydrodynamic waves [Lee, 1983]. More recently, attention has been drawn to the notable flattening of proton energy spectra in observations directly preceding the passage of interplanetary shocks at Earth [Lario *et al.*, 2018]. This is attributed to the propagation of accelerated particles from the shock to the observer, but, the mechanisms are however not fully explained. Moreover, while CME shock properties such as speed and compression ratio have been linked to the efficiency of particle acceleration [Lario *et al.*, 2005b; Giacalone, 2012], shock obliquity [Ellison *et al.*, 1995], and the nature of the seed particles [Desai *et al.*, 2006] have also been identified as important factors. Injection into the DSA process is facilitated by the formation of non-thermal seed particles [Neergaard-Parker *et al.*, 2014; Zank, 2017], which has also been investigated using kinetic hybrid simulations [Caprioli *et al.*, 2015; Sundberg *et al.*, 2016].

In this chapter, two broad scientific questions are addressed, namely, how the prior heating of the SW distribution affects acceleration at interplanetary shocks, and what role these shock-accelerated particles play in producing the spectral features observed during ESP events. The acceleration of SW particles is modelled by solving a set of SDEs equivalent to the *Parker* [1965a] TPE in spherical symmetry. The applications are limited to halo CME shocks expanding radially at constant speeds. In this spherically symmetrical scenario, the shock normal is radially aligned so that the shock obliquity can be approximated using the *Parker* [1958] spiral angle. It is firstly considered how the initial SW distribution transforms in response to changes in the plasma properties (Section 4.3.2), and later how the resulting distribution affects the subsequent DSA process as a seed population (Section 4.6). The classical spectral characteristics of DSA for travelling shocks and the comparative efficiency of DSA at fast and strong shocks are revisited in Sections 4.4 and 4.5, respectively. In addition to reproducing these more typical

DSA features, the model is also applied to investigate the spectral flattening reported by *Lario et al.* [2018] ahead of interplanetary shock passages (Section 4.6.2), as well as to identify the original spatial distributions and energies of seed particles that would eventually contribute to intensities during ESP events (Section 4.6.3).

This chapter is largely based on the content of *Prinsloo et al.* [2019].

4.2 Modelling energetic particle acceleration at CME shocks

The events of interest in this chapter are large ESP events with small associated anisotropies. These events are typically associated with fast-moving shocks driven by halo CMEs [*Mäkelä et al.*, 2011], that is, those propagating radially outward and approximately centred on the solar disk. Therefore, to describe the transport and DSA of energetic particles associated with such events, it is sufficient to solve the *Parker* [1965a] transport equation (TPE) for a single spatial dimension. See also the motivation offered by *Giacalone* [2015] in this regard. Hence, in radial coordinates, the TPE of Eq. 3.23 simplifies to

$$\frac{\partial f}{\partial t'} = \left(\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \kappa_{rr}) - V_{sw}' \right) \frac{\partial f}{\partial r} + \kappa_{rr} \frac{\partial^2 f}{\partial r^2} + \frac{1}{3r^2} \frac{d(r^2 V_{sw}')}{dr} E \xi(E) \frac{\partial f}{\partial E} + Q, \quad (4.1)$$

with $\xi(E) = (E + 2E_p)/(E + E_p)$, where E_p is the proton rest-mass energy. When presented, the distribution function is converted to units of differential intensity, that is, $j = p^2 f$. The diffusion coefficient considered is the effective radial diffusion coefficient κ_{rr} , which relates to the equivalent mean free path (MFP) λ_{rr} according to

$$\kappa_{rr} = \frac{v}{3} \lambda_{rr}, \quad (4.2)$$

where v is the particle speed and λ_{rr} is given by

$$\lambda_{rr} = \lambda_0 \left(\frac{R}{R_0} \right)^{1/3} \quad (4.3)$$

where $R = \sqrt{E^2 + 2EE_p}$ is the particle rigidity and λ_0 is a reference MFP defined at 1 GeV. Given that the parallel diffusion coefficient is much larger than the perpendicular coefficient, and magnetic field lines are largely radial for the fast flow speeds considered, diffusion along field lines is assumed to dominate. The rigidity dependence implemented here is thus chosen to emulate that predicted for parallel diffusion by quasi-linear theory [*Jokipii*, 1966] for a Kolmogorov-range turbulence power spectrum [*Bieber et al.*, 1994]. *Kallenrode et al.* [1992] reports no pronounced variation in MFPs with radial distance between the Sun and 1 AU for diffusive events. As such, a radial dependence is omitted in Eq. 4.3. Furthermore, radial MFPs of 0.02 to 0.15 AU are reported for 0.3 to 0.8 MeV electrons [*Kallenrode et al.*, 1992], and the ratio of MFPs for 18 MeV protons to 1 MeV electrons as 1.6 ± 0.9 [*Kallenrode*, 1993]. Taking the lower limits of the aforementioned quantities into account, the corresponding lower limit of λ_0 (defined at 1 GeV) for protons is estimated from Eq. 4.3 as ~ 0.05 AU. λ_0 is varied in Section 4.4 and chosen as 0.06 AU elsewhere, using the above lower limit and the results of the aforementioned

section as guidelines.

4.2.1 A spherically symmetrical SDE model

The TPE is solved numerically using the SDE-approach detailed in Section 3.4. Eq. 4.1 is conveniently written in the form of the time-backward Kolmogorov equation

$$-\frac{\partial f}{\partial t} = \mu_r \frac{\partial f}{\partial r} + \mu_E \frac{\partial f}{\partial E} + \frac{1}{2} \sigma_r^2 \frac{\partial^2 f}{\partial r^2}, \quad (4.4)$$

from which the SDEs can be cast into the form of the Itô equation [see *e.g.* Zhang, 1999]

$$dr = \mu_r dt + \sigma_r dW \quad (4.5)$$

$$dE = \mu_E dt, \quad (4.6)$$

where $dW = \sqrt{dt} \Lambda(t)$ represents the Wiener process and $\Lambda(t)$ is a simulated Gaussian-distributed pseudo-random number. Substituting the coefficients corresponding to μ_r , μ_E , and σ_r from Eq. 4.1 into Eqs. 4.5 and 4.6 yields

$$dr = \left(\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \kappa_{rr}) - V'_{sw} \right) dt + \sqrt{2\kappa_{rr} dt} \Lambda(t) \quad (4.7)$$

$$dE = \frac{1}{3r^2} \frac{d(r^2 V'_{sw})}{dr} E \xi(E) dt, \quad (4.8)$$

which are equivalent to the TPE in Eq. 4.1. These SDEs are integrated in a time-backwards fashion. Starting from an observational point $(r_{\text{obs}}, E_{\text{obs}})$ at which the value of the distribution function is sought, Eqs. 4.7 and 4.8 are solved iteratively using the Euler-Maruyama numerical scheme [Maruyama, 1955] for a finite time step Δt . The coordinates r and E are updated after each iteration until $t' = 0$, or equivalently, until $t = t_T$.

When simulating ESP events, t_T is chosen as the transit time of the shock travelling (in a time-backwards fashion) from r_{obs} to the inner modulation boundary near the Sun ($r_{\text{min}} = 5r_{\odot}$), that is, $t_T = (r_{\text{obs}} - r_{\text{min}})/V_{sh}$. The shock position r_{sh} is therefore updated in step with r and E , according to

$$r_{sh} = r_{\text{obs}} - V_{sh} t \quad (4.9)$$

where $0 < t \leq t_T$. A constant shock speed is assumed, since the mean acceleration of CME-driven shocks associated with ESP events is reportedly close to zero [Mäkelä *et al.*, 2011]. As discussed in Section 3.4, the time is incremented variably, depending on the dominant transport process at the current position, to maintain a fixed step length, such that

$$\Delta t = \min \left\{ \frac{0.1L}{\max \left(\left| \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \kappa_{rr}) \right|, V'_{sw} \right)}, \frac{0.1L^2}{\kappa_{rr}} \right\}, \quad (4.10)$$

for the spherically symmetrical case. Finally, a reflective inner boundary is implemented such that if $r < r_{\text{min}} \implies r = 2r_{\text{min}} - r$, while at the outer boundary, if $r > r_{\text{max}} = 1.4 \text{ AU}$,

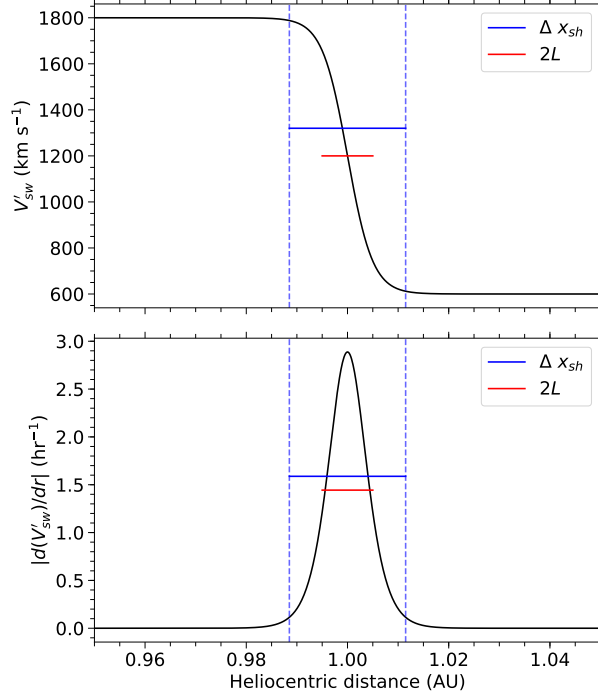


Figure 4.1: Top: An example of the transition of the fixed-frame SW flow speed V'_{sw} as a function of heliocentric distance r with the shock centred at Earth, $r_{sh} = 1$ AU. Bottom: Absolute value of the gradient of V'_{sw} corresponding to the profile shown above. The quantities L ($= 0.005$ AU) and Δx_{sh} are as later defined for Eq. 4.12 and Eq. 4.13, respectively.

the time-integration routine is interrupted and that pseudo-particle's contribution is discarded, defining an absorbing boundary condition. Note that simulated intensities of shock-accelerated particles at Earth were mostly insensitive to variations in the outer boundary location beyond $r_{\max} \sim 1.2$ AU. This likely follows because the most significant contributions to intensities were found to originate from upwind of 1 AU as discussed in Section 4.6.3.

4.2.2 Modelling the shock source function

As per Eq. 3.32, when a pseudo-particle is traced back to a point where it interacts with the shock, its amplitude is attributed a value that depends on the product of the source function Q and the time Δt it spends interacting with the shock. Indeed, considering Eq. 4.1, Q should have units corresponding to that of the distribution function per unit time. Otherwise, the specification of Q is largely arbitrary: *e.g.* Giacalone [2015] employs delta functions, others [*e.g.* le Roux *et al.*, 1996] specify distribution functions to represent seed populations, whereas Malkov and Voelk [1995] also consider shock-heated seed populations. Drawing on aspects of the aforementioned examples, the following source function is proposed:

$$Q = \frac{f_{\kappa}}{m_p^3} \left| \frac{dV'_{sw}}{dr} \right| H \left(\frac{E - E_{\text{inj}}}{E_{\text{inj}}} \right). \quad (4.11)$$

Here, f_{κ} is the κ -function representing the SW distribution. As discussed in Appendix A, the m_p^3 factor is included for dimensional consistency between f_{κ} and the distribution function in the TPE. Since f_{κ} is already normalised to the number density, scaling the SDE solutions is

not necessary. The dimensionless Heaviside function $H((E - E_{\text{inj}})/E_{\text{inj}})$ ensures that only the contributions of particles with energies larger than the injection energy E_{inj} are included. Note that $E_{\text{inj}} = 60$ keV unless stated otherwise (see also Section 4.6.1). The absolute value of the SW velocity gradient $|dV'_{sw}/dr|$ is included to provide a spatial region with a width and position that is self-consistently associated with the shock and that has a reasonable probability of being sampled by pseudo particles. Figure 4.1 shows how $|dV'_{sw}/dr|$ is representative of the width of the shock. While it is sufficient for a physical particle to pass between the upstream and downstream media in order to gain energy, using this time-backward SDE method requires a finite-width region to be sampled by pseudo particles to register flux emanating from the shock.

4.3 Modelling the solar wind energy distribution

The κ -function introduced in Eq. 2.5 is used to represent the SW energy distribution. It is incorporated into the numerical model by means of the source function as specified in Eq. 4.11. An objective of this study is to consider how the κ -function changes during the passage of an interplanetary shock, and to implement this transformed distribution as a seed-particle spectrum for DSA.

4.3.1 Transitions of plasma properties across travelling shocks

To study the evolution of the SW energy distribution, it is necessary to model the changes in n and T , upon which f_κ depends [see also *Livadiotis, 2015*]. Note that the κ -index is assumed to remain constant across the shock. For consistency, transitions across the shock are modelled to correspond to that of the flow speed that would be observed by *e.g.* a spacecraft in Earth's orbit. The SW is modelled to transition between upstream and downstream flow speeds in the spacecraft (or fixed) frame, given as $V'_1 (= \text{constant})$ and $V'_2 = (V_{sh}(s - 1) + V'_1)/s$ respectively, according to

$$V'_{sw} = \frac{1}{2s} \left(V'_1(s + 1) + V_{sh}(s - 1) - (s - 1)(V_{sh} - V'_1) \tanh \left(\frac{r - r_{sh}}{L} \right) \right), \quad (4.12)$$

where s is the shock compression ratio (or ratio of up and downstream flow velocities in the shock frame), V_{sh} is the shock speed, $r - r_{sh}$ is the radial position relative to the position of the shock r_{sh} , and L is a characteristic length used to specify the broadness of this transition. The derivation of the downstream fixed-frame flow speed V'_2 is discussed in Appendix C. Figure 4.2 illustrates this transition for the reference parameters listed in Table 4.1. Should $V_{sh} = 0$, Eq. 4.12 reduces to an expression [used by *e.g. le Roux et al., 1996*] for a stationary shock. Note furthermore that L is not a direct measure of the shock width. Its extent can however be approximated from Eq. 4.12 as $\Delta x_{sh} \approx 2r_c$ with

$$r_c = \tanh^{-1} \left(\frac{2sV_c - V'_1(s + 1) - V_{sh}(s - 1)}{(1 - s)(V_{sh} - V'_1)} \right) L, \quad (4.13)$$

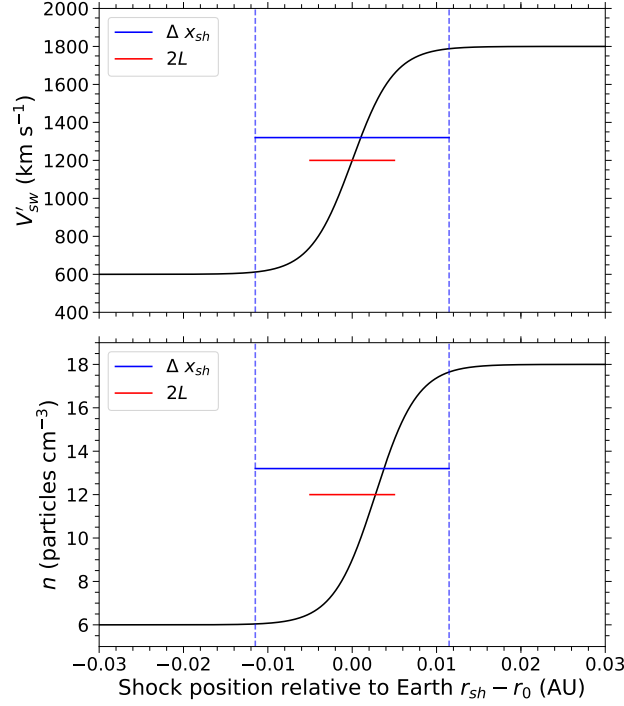


Figure 4.2: Top: The transition of the fixed-frame SW flow speed V'_{sw} , as viewed by an observer at the Earth, as a function of the shock position relative to that of the Earth ($r_{sh} - r_0$). L ($= 0.005$ AU) and Δx_{sh} are as defined for Eq. 4.12 and Eq. 4.13, respectively. Bottom: The SW number density profile corresponding to the flow-speed profile shown above.

V'_{sw} :	V'_1	600	km s^{-1}
	V_{sh}	2400	km s^{-1}
	s	3.0	
	L	0.005	AU
n :	n_0	6.0	cm^{-3}
T :	T_e	5×10^5	K
	γ_c	5/3	
f_κ :	κ	2.25	

Table 4.1: Reference configuration of the parameters needed to define the fixed-frame flow speed V'_{sw} , number density n , temperature T and κ -function as discussed in Section 4.3.1.

where a fraction $\mathcal{C} \in [0, 0.5]$ is chosen such that $V_c = V'_1 + \mathcal{C}(V'_2 - V'_1)/2$ is the flow speed at some distance r_c from the shock. Typically, to approximate the shock width, $\mathcal{C} = 0.01$ so that $V_c \approx V'_1$. It is illustrated in Figure 4.2 how the lengths Δx_{sh} , L , and the actual shock width compare with one another.

With the flow speed transition given, the change in number density n across the shock follows from the continuity equation. Of course, the total factor by which the number density jumps across the shock must be equal to the compression ratio. In terms of V'_{sw} it follows, in spherical coordinates, that

$$n = n_0 \frac{V_{sh} - V'_1}{V_{sh} - V'_{sw}} \left(\frac{r_0}{r} \right)^2, \quad (4.14)$$

where n_0 is the number density at some reference position such as the Earth ($r_0 = 1$ AU), and where the flow speeds are transformed back to the shock frame, their ratio being equal to s . This transition is also shown in Figure 4.2.

To estimate the jump in temperature across the shock, instead of implementing the relevant hydromagnetic Rankine-Hugoniot jump condition, a simpler approach capturing the essential physics is used. The magnetic energy is expected to be much smaller than the thermal energy in the flow-dominated region considered in this study. It is therefore assumed that the change in kinetic energy density $d\mathcal{E}_{sw}$ of the bulk solar wind flow, as a function of position through the shock, is converted to thermal energy. That is,

$$d\mathcal{E}_{sw} = \frac{1}{2}m_p \left(n_0 (V_1' - V_{sh})^2 - n (V_{sw}' - V_{sh})^2 \right), \quad (4.15)$$

which is related through the equipartition theorem to the change in temperature dT_{sw} by

$$dT_{sw} = \frac{2}{\mathcal{N}_{df}} \frac{d\mathcal{E}_{sw}}{nk_b}, \quad (4.16)$$

where $\mathcal{N}_{df} = 2/(\gamma_c - 1)$ is the number of degrees of freedom and γ_c is the ratio of specific heats. dT_{sw} is subsequently added to the unshocked temperature value, $T = T_0 + dT_{sw}$, where

$$T_0 = T_e (r/r_0)^{2(1-\gamma_c)} \quad (4.17)$$

and T_e is the plasma temperature at the Earth. For a monatomic gas for which $\gamma_c = 5/3$ it follows that $T_0 \propto r^{-4/3}$. It is assumed that the temperature gain during the shock passage is not significant enough to disassociate molecules, and hence γ_c remains constant as for a calorically ideal gas. Furthermore, given the multi-species composition of the SW plasma, γ_c may deviate from the monatomic value of $5/3$. It is noted that while the hydromagnetic treatment of the shock jump conditions may break down in the transition region itself, it approximates the up and downstream quantities adequately. As also shown in Section 4.4.1, DSA requires particles to interact with the shock at length scales exceeding its width [e.g. Jones and Ellison, 1991; Kruells and Achterberg, 1994]. This description is thus sufficient for the present study.

The shock transitions of V_{sw}' , n and T are displayed in the left panel of Figure 4.3 as viewed by an observer at Earth's position. The parameters used to define these quantities are listed in Table 4.1 and are mostly informed by observations of CMEs during the 2003 Halloween epoch [Skoug et al., 2004; Richardson et al., 2005; Gopalswamy et al., 2005; Lario et al., 2005a; Wu et al., 2005]. In particular, SW flow speeds in excess of 1800 km s^{-1} [Skoug et al., 2004] and shock speeds of $\sim 2400 \text{ km s}^{-1}$ [Gopalswamy et al., 2005; Wu et al., 2005] are noted. Since density measurements during some larger events were uncertain [e.g. Skoug et al., 2004; Wu et al., 2005], the compression ratio for such events can be calculated using the ratios of shock-frame flow velocities. For example, $s = (V_{sh} - V_1')/(V_{sh} - V_2') = 3$ for $V_{sh} = 2400 \text{ km s}^{-1}$, $V_1' = 600 \text{ km s}^{-1}$ and $V_2' = 1800 \text{ km s}^{-1}$.

4.3.2 Evolution of the κ -function during the shock passage

Aside from κ , which is kept fixed, f_κ is shown in Section 2.5 to depend on parameters n and T , both of which change during the shock passage. Additionally, to illustrate how the SW distribution evolves when the flow speed is shocked to higher values, it is necessary to express

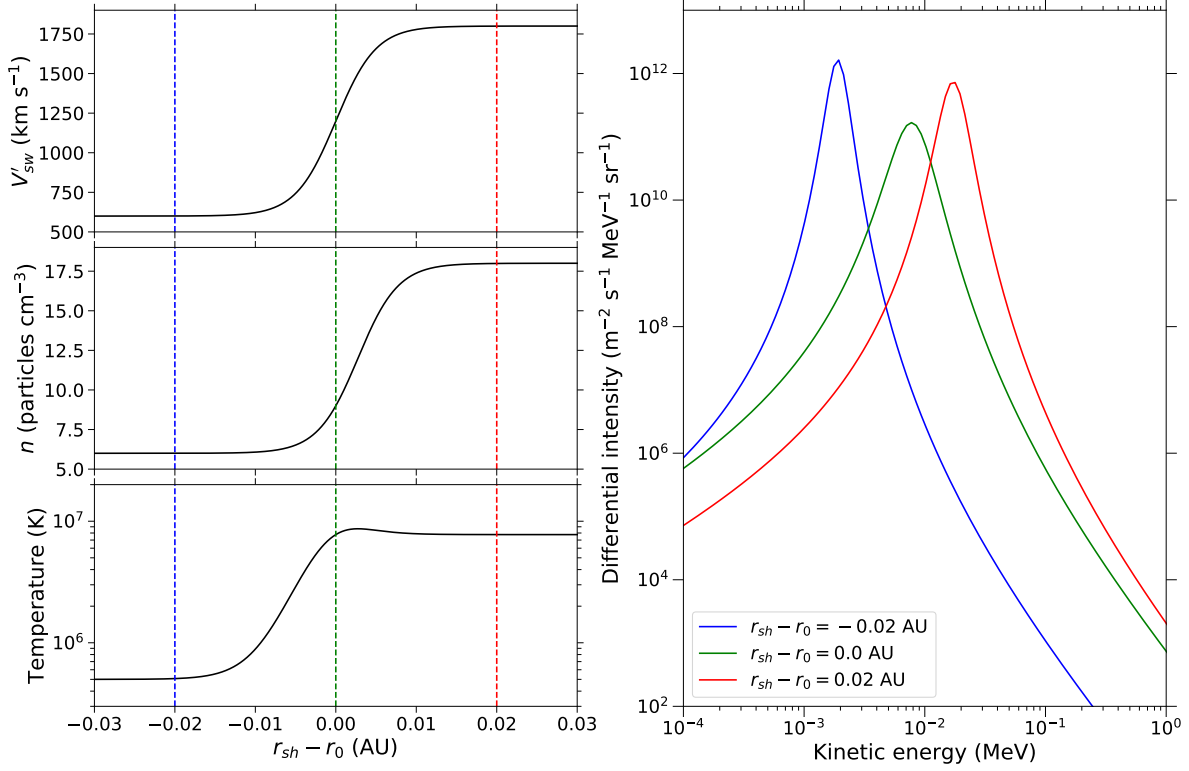


Figure 4.3: Left: The transitions of the fixed-frame SW flow speed V'_{sw} , number density n , and temperature T , as viewed by an observer at the Earth, as a function of the shock position relative to that of the Earth ($r_{sh} - r_0$). Right: The heating of the SW energy distribution at the Earth in response to the shock transitions of plasma parameters as shown on the left. The curves represent SW distributions at different stages of the shock passage corresponding with the values of $r_{sh} - r_0$ indicated using vertical lines of similar colors on the left.

the particle speed in f_κ relative to the flow speed in the spacecraft frame, that is, $v \rightarrow v - V'_{sw}$ [see also *Leubner, 2004; Kong et al., 2017*]. The SW distribution is therefore expected to be transformed by the shock in at least three ways, depending on how V'_{sw} , n , and T change. To illustrate this transformation, the SW distribution, as represented by f_κ and viewed by an observer at Earth, is shown at different stages during the shock passage on the right-hand side of Figure 4.3 for parameters as specified in Table 4.1. Bear in mind that these distributions have not yet been injected into the DSA process, and that these transformations occur solely because the shock had heated the SW plasma. Also note that for consistency with the units in which observations are typically presented, f_κ is converted throughout this study into units of differential intensity (as discussed in Section 3.2.2) and is subsequently denoted as j_κ .

While the shock is still 0.02 AU away from the Earth, Figure 4.3 shows that the SW distribution at Earth will remain unchanged since none of the plasma quantities have been shocked at this point. When the shock passes Earth, when $r_{sh} = r_0$, the temperature is shown to have increased substantially, accompanied by more modest increases in the flow speed and density. The most obvious changes incurred by the SW distribution at this point are that it notably broadened as a result of the temperature increase, and that the thermal peak shifted to higher energies as a result of the increased flow speed. Note that because f_κ is normalised to the number density, the conservation of particles demands that the peak intensity of the distribution decreases when it broadens. Lastly, when the shock has moved 0.02 AU beyond the Earth, the SW distribution

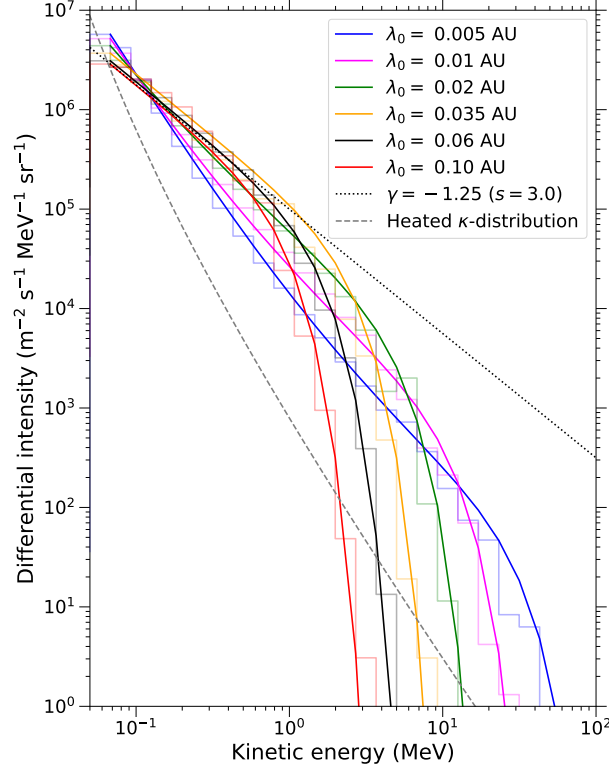


Figure 4.4: Modelled energy spectra at the Earth ($r = 1$ AU) at the time of the shock passage for different values of λ_0 . Step-like lines represent SDE solutions, while the smooth solid lines are corresponding fits of Eq. 4.20 using the parameters listed in Table 4.2. Also included are the heated κ -distribution (dashed grey line), specified as a source function on the shock, and the $E^{-1.25}$ power law associated with a shock compression ratio of $s = 3$ (dotted line).

shifts further, to higher energies, as the flow speed attains its full downstream value. This is accompanied by increasing overall intensities due to the increase in number density. At this point the temperature has already plateaued and hence the distribution shows no appreciable broadening from when the shock passed Earth's position.

4.4 Spectral features of shock-accelerated particles.

The most distinctive characteristics of shock-accelerated particles are observed in their energy spectra, which are considered here at the time the shock passes an observer near the Earth. Implementing the model configuration discussed in Sections 4.2 and 4.3, and scaling the diffusion coefficient by varying the value of λ_0 in Eq. 4.3, the dependence of shock-accelerated spectral features on this transport process is investigated. The resultant spectra are shown in Figure 4.4.

Qualitatively, the typical DSA-associated features are evident: a power-law distribution at lower energies transitioning to an exponential-like decrease at higher energies [Ellison and Ramaty, 1985]. This distribution can be described using a simple function of the form,

$$j_{\text{DSA}} = j_0 \left(\frac{E}{E_0} \right)^{\gamma_s} e^{-(E/E_{\text{cut}})^2}, \quad (4.18)$$

where j_0 is a differential intensity defined at some reference energy E_0 , E_{cut} is the cut-off (or

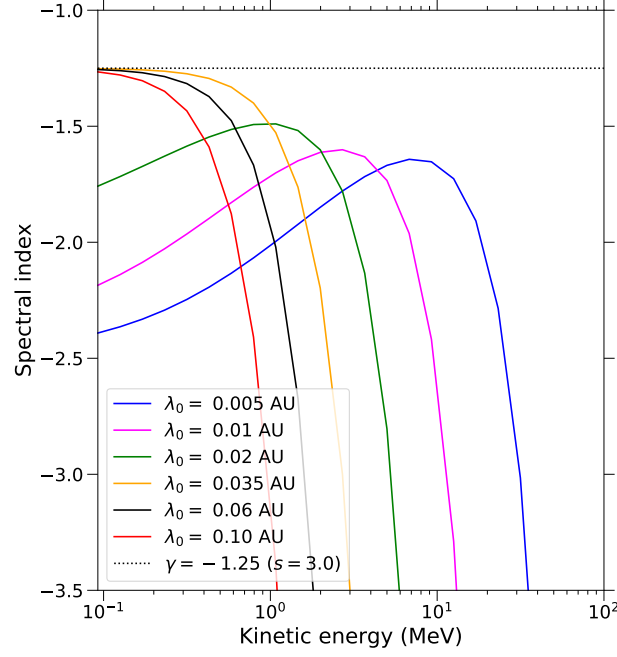


Figure 4.5: Spectral indices for the corresponding fits of Eq. 4.20 shown in Fig. 4.4. The spectral index $\gamma_s = -1.25$ for a shock with $s = 3$ is also shown.

λ_0 (AU)	γ_a	E_{tr} (MeV)	E_{cut} (MeV)
0.005	-2.5	1.5	30.0
0.01	-2.4	0.5	11.0
0.02	-2.0	0.2	5.0
0.035	-1.25	0.08	2.5
0.06	-1.25	-	1.5
0.1	-1.25	-	0.9

Table 4.2: Parameters used to fit Eq. 4.20 to the corresponding model solutions shown in Figure 4.4. The λ_0 -values are constants used to scale the MFPs in Eq. 4.3. E_{tr} and E_{cut} are energies at which spectra transition to power-law indices associated with the full shock compression and roll over into exponential decreases, respectively. γ_a is the spectral index for $E < E_{\text{tr}}$. Note that E_{tr} -values are omitted for the two largest λ_0 -values, because $\gamma_a = \gamma_b = -1.25$ in these scenarios, which reduces Eq. 4.20 to the form of Eq. 4.18.

roll-over) energy above which the distribution begins to decrease exponentially, and where

$$\gamma_s = \frac{s+2}{2-2s} \quad (4.19)$$

is the spectral index (for $E \ll E_p$) associated with the compression ratio s of the shock [see also Ellison *et al.*, 1990]. For $s = 3$, as specified for these solutions, it is therefore expected that $\gamma_s = -1.25$. However, not all of the spectra in Figure 4.4 appear to follow a $E^{-1.25}$ power law. This is accentuated in Figure 4.5, which shows spectral indices for solutions with smaller λ_0 -values actually varying with energy even before the exponential decreases occur. To describe this behaviour, it is useful to generalise Eq. 4.18 as follows:

$$j_{\text{DSA}} = j_0 \left(\frac{E}{E_0} \right)^{\gamma_a} \left(\frac{E^\xi + E_{\text{tr}}^\xi}{E_0^\xi + E_{\text{tr}}^\xi} \right)^{(\gamma_b - \gamma_a)/\xi} e^{-(E/E_{\text{cut}})^2}. \quad (4.20)$$

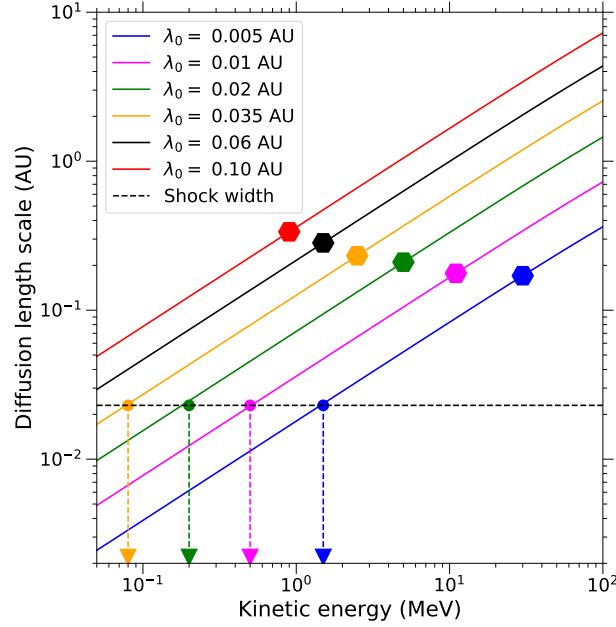


Figure 4.6: Diffusion length scales at the shock, calculated using Eq. 4.21 and corresponding to the solutions shown in Figure 4.4. Varying λ_0 -values scales the energy profiles of κ_{rr}/V_{sw} uniformly. Markers indicate the values of κ_{rr}/V_{sw} at the corresponding cut-off energies (E_{cut}) listed in Table 4.2. Arrows indicate the energies E_{tr} (also listed in Table 4.2) at which the respective κ_{rr}/V_{sw} profiles are equal to the shock width (dashed horizontal line), which is calculated using Eq. 4.13.

This describes a function transitioning between power-law indices γ_a and γ_b about E_{tr} , with ξ specifying the smoothness of this transition, and which rolls over into an exponential decrease above E_{cut} . Note that if $\gamma_a = \gamma_b$, this expression simplifies to the form of Eq. 4.18. Setting $\gamma_b = \gamma_s$, where $\gamma_s = -1.25$ for $s = 3$, and choosing $\xi = 0.8$, the function given in Eq. 4.20 is fitted to the solutions in Figure 4.4 with parameters as presented in Table 4.2.

Both γ_a and E_{cut} respond to varying the value of λ_0 , affecting both the hardness of the spectra and the energies up to which they are accelerated. The behaviour of these two sets of features and the underlying physics are discussed separately in the subsections below.

4.4.1 On shock widths and diffusion length scales

Classically, the spectral index associated with a DSA-produced spectrum is a function of the shock compression ratio alone. The behaviour observed in Figure 4.4, where shock-accelerated spectra become softer, displaying smaller spectral indices for smaller diffusion coefficients, is therefore not theoretically expected. Note, however, that the solutions for $\lambda_0 \geq 0.035$ AU do follow the theoretically predicted power law of $E^{-1.25}$ for $s = 3$. Figure 4.5 shows the spectral indices of the solutions presented in Figure 4.4. Here, spectral indices are also shown to be equal to -1.25 for large λ_0 -values at low energies. Indices become progressively smaller for smaller λ_0 -values, but increase toward higher energies. Consider that particles with $\lambda_0 \lesssim 0.035$ AU may be sampling only a fraction of the total compression of the shock. The spectra harden toward higher energies, because the MFPs themselves increase with energy and progressively greater fractions of the total compression are sampled.

This effect is illustrated in Figure 4.6. Recall from Eq. 4.2 that $\kappa_{rr} \propto \lambda_{rr}$, which is scaled using

λ_0 . Since κ_{rr} does not have dimensions of length, when comparing to other length scales it is useful to define the diffusion length scale κ_{rr}/V_{sw} , which is often expressed as the sum of the up and downstream values at the shock [e.g. *Steenberg and Moraal, 1999*]. That is,

$$\begin{aligned} \left(\frac{\kappa_{rr}}{V_{sw}} \right)_{(r=r_{sh})} &= \left(\frac{\kappa_{rr}}{V_{sw}} \right)_1 + \left(\frac{\kappa_{rr}}{V_{sw}} \right)_2 \\ &= \kappa_{rr} \left(\frac{1}{V_1} + \frac{1}{V_2} \right), \end{aligned} \quad (4.21)$$

where $(\kappa_{rr})_1 = (\kappa_{rr})_2 = \kappa_{rr}$, since κ_{rr} is assumed not to change across the shock, with subscripts 1 and 2 denoting up and downstream values, respectively. Here, $V_1 = V_{sh} - V'_1$ and $V_2 = (V_{sh} - V'_1)/s$ are the up and downstream flow speeds in the shock frame. This quantity is plotted as a function of energy in Figure 4.6, along with the shock width, calculated using Eq. 4.13 for $L = 0.005$ AU. Note that for $\lambda_0 = 0.06$ and 0.1 AU, for which spectra are aligned with $E^{-1.25}$, the diffusion length scales are greater than the shock width for all energies in the considered domain. Those particles therefore sample the full compression ratio, and hence their energy distributions display the power law associated with $s = 3$. A similar effect is reported for the heliospheric termination shock [e.g. *Arthur and le Roux, 2013*]. For $\lambda_0 < 0.06$ AU, particles sample fractional compression ratios up to the energies where their respective diffusion length scales begin to exceed the shock width. Indeed, the energies at which κ_{rr}/V_{sw} and the shock width intersect provide good estimates for E_{tr} in Table 4.2.

Since the prediction of DSA given in Eq. 4.19 is only observed where κ_{rr}/V_{sw} is larger than the width of the shock, these results are in agreement with the length scale hierarchy of $\kappa_{rr}/V_{sw} \gg \lambda_{rr} \gg \Delta x_{sh}$ required for classical DSA to be valid [*Blandford and Ostriker, 1978; Jones and Ellison, 1991*]. Given the L -dependence of the variable time step (Eq. 4.10), to limit computation times, the shock width in this study is chosen to be much broader ($L = 0.005$ AU) than typical interplanetary shock widths [$L \sim 10^{-6}$ AU; e.g. *Sapunova et al., 2017*]. Nevertheless, the results of the model should remain valid as long as the aforementioned length scale hierarchy is observed.

4.4.2 Finite-time acceleration and the termination of shock-accelerated spectra

The second set of features considered pertains to the highest energies attained by accelerated spectra before intensities begin to decrease exponentially. Figure 4.4 illustrates that spectra for smaller λ_0 -values are accelerated to higher energies before terminating. These energies, represented by E_{cut} , are listed in Table 4.2. Since they notably respond to varying λ_0 , it seems reasonable to expect that this spectral transition also occurs due to κ_{rr}/V_{sw} attaining some characteristic length. Shock-accelerated spectra have previously been reported to roll over due to diffusion length scales becoming comparable to system sizes or some related length of the shock geometry [*Ellison and Ramaty, 1985; Steenberg and Moraal, 1999*]. Indeed, Figure 4.6 shows the diffusion length scales corresponding to each of the cut-off energies of the solutions in Figure 4.4 are reasonably similar, distributed between 0.1 and 0.4 AU. However, these do not resemble any obvious length scale in either the physical system or within the numerical model. Simulations where the position of modulation boundaries were varied yielded negligible effects on energy spectra, suggesting that system size is not the limiting factor in this instance.

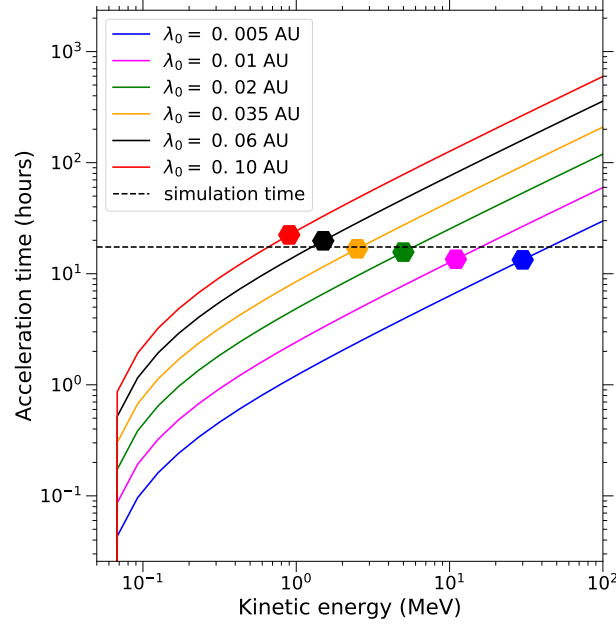


Figure 4.7: Acceleration time as function of kinetic energy, calculated using Eq. 4.22, for the corresponding diffusion length scale profiles shown in Figure 4.6. Markers indicate the time required to accelerate spectra up to the corresponding cut-off energies (E_{cut}) listed in Table 4.2. The simulation time (horizontal line) is the time taken by the shock to travel from near the Sun to Earth at 2400 km s^{-1} .

Another instructive quantity that is related to the diffusion length scale is the acceleration time [Drury, 1983; Ellison *et al.*, 1990], which is the time required to accelerate particles from a particular energy (or equivalent momentum) to another at a planar shock. This is expressed in terms of the diffusion length scale as

$$\tau_a = \frac{3}{V_1 - V_2} \int_{p_{\text{inj}}}^p \kappa_{rr} \left(\frac{1}{V_1} + \frac{1}{V_2} \right) \frac{dp'}{p'}, \quad (4.22)$$

where V_1 and V_2 are as defined for Eq. 4.21 and p_{inj} is the momentum equivalent to E_{inj} . Note that momentum is generally related to kinetic energy according to $p = (1/c)\sqrt{E^2 + 2EE_p}$ (for protons), where E_p is the proton rest-mass energy. Eq. 4.22 is used in Figure 4.7 to approximate the time required to accelerate spectra up to different energies for each of the length scale profiles shown in Figure 4.6. Also shown in Figure 4.7, as hexagonal markers, are the times required to accelerate spectra up to the observed cut-off energies listed in Table 4.2 for each respective κ_{rr}/V_{sw} -profile.

Similar to the diffusion length scales, the acceleration times corresponding to each of the cut-off energies have comparable values. These τ_a -values also compare well to the total duration of the simulation, which is equal to the time taken by the shock to travel from near to the Sun to Earth at 2400 km s^{-1} , that is, ~ 17.3 hours. This suggests that for each spectrum in Figure 4.4, E_{cut} is the highest energy that could be attained in the available time [see also Channok *et al.*, 2005; Kong *et al.*, 2019]. At $E > E_{\text{cut}}$, the rate of escape of particles from the shock begins to exceed the acceleration rate, which leads to the observed exponential intensity decreases. In this context, smaller diffusion coefficients serve to better confine particles near the shock. This reduces the time required to accelerate particles up to a particular energy, or stated differently,

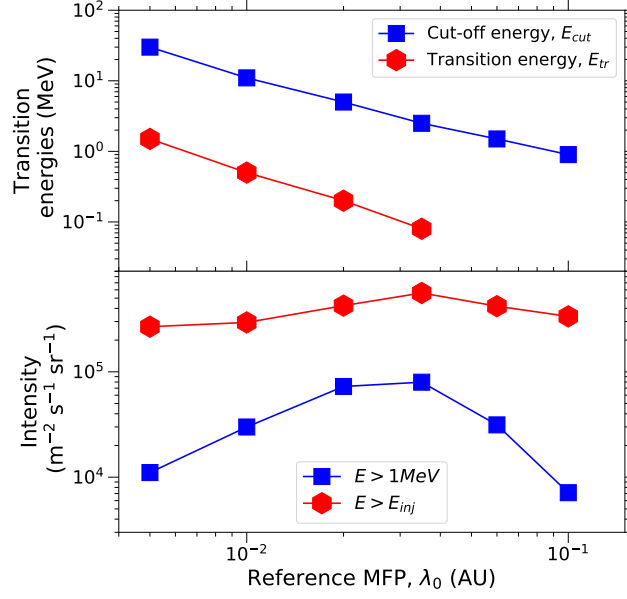


Figure 4.8: Top: Energies E_{tr} and E_{cut} at which spectra for different values of λ_0 transition to power-law indices associated with the full compression and roll over into exponential decreases, respectively. Bottom: The energy-integrated distributions for different values of λ_0 as a measure of how efficiently DSA produces particles above the injection energy and 1 MeV, respectively.

allows particles to be accelerated to higher energies within the available time.

4.4.3 Spectral features and acceleration efficiency

The preceding discussions reveal that the characteristics of shock-accelerated spectra are sensitive to the values of diffusion length scales in two opposing ways: Diffusion length scales should exceed shock widths for spectra to display DSA-predicted power-law indices, but accelerated spectra terminate at lower energies for larger diffusion length scales. The top panel of Figure 4.8 illustrates this dichotomy. The energies E_{tr} , above which κ_{tr}/V_{sw} exceeds the shock width, become smaller with increasing λ_0 -values, implying greater overall spectral hardening. Similarly, decreasing E_{cut} -values imply that spectra terminate at lower energies. Harder spectra yield larger intensities of energetic particles, but so do higher cut-off energies. Yet, with regards to diffusion properties, they are attained in opposite ways. Neither of these therefore necessarily provide meaningful measures of acceleration efficiency on their own.

To evaluate which combination of spectral features yield greater intensities of energetic particles, it is useful to consider particle fluences. These are calculated by integrating differential intensities over energy as follows:

$$I_{E_l} = \int_{E_l}^{\infty} j(E) dE. \quad (4.23)$$

This integral converges, since j always decreases as $E \rightarrow \infty$. Eq. 4.23 is evaluated for each of the spectra shown in Figure 4.4 with two different lower limits, namely $E_l = E_{inj}$ and 1 MeV. The resulting energy-integrated intensities are shown in the bottom panel of Figure 4.8. The total intensity for all particles with $E > E_{inj}$ peaks at $\lambda_0 \sim 0.035$ AU, where the power-law segments of spectra have reached, or nearly reached, their maximum hardness. The quantity E_{cut}

	V_{sh} (km s ⁻¹)	s	V_2 (km s ⁻¹)	V_2' (km s ⁻¹)	V_2'/V_1'
1:	3000	3	800	2000	3.67
	2800	3	733	2067	3.44
	2600	3	667	1933	3.22
	2280	3	560	1720	2.87
	2200	3	533	1667	2.78
2:	2400	2	900	1500	2.5
	2400	2.2	818	1581	2.64
	2400	2.5	720	1680	2.8
	2400	3.5	514	1886	3.14
	2400	4	450	1950	3.25
3:	3000	2	1200	1800	3
	2800	2.2	1000	1800	3
	2600	2.5	800	1800	3
	2280	3.5	480	1800	3
	2200	4	400	1800	3
ref:	2400	3	600	1800	3.0

Table 4.3: Configurations used throughout Section 4.5, in which 1: the shock speed V_{sh} is varied, 2: the compression ratio s is varied, and 3: V_{sh} and s are varied together such that V_2'/V_1' remains constant. Here, $V_1' = 600$ km s⁻¹ and $V_2' = (V_{sh}(s - 1) + V_1')/s$ are the fixed-frame flow speeds, respectively up and downstream of the shock. $V_2 = (V_{sh} - V_1')/s$ is the downstream flow speed in the shock frame. The last line contains the reference configuration.

becomes more important when considering higher-energy particles. For intensities integrated upward from 1 MeV, fluences peak between $\lambda_0 = 0.02$ and 0.035 AU and notably decrease for larger λ_0 -values due to spectra rolling over at lower energies.

Both spectral hardness and the maximum energies of spectra therefore contribute to the number of energetic particles DSA is able to produce. Of course, the energies up to which spectra extend become increasingly important for the intensities of higher-energy particles.

4.5 Strong shocks versus fast shocks

Fast-moving CME shocks with large compression ratios are reported to be more efficient at accelerating energetic particles [Lario *et al.*, 2005b; Mäkelä *et al.*, 2011; Giacalone, 2012]. How conducive each of these shock properties are to producing large numbers of high-energy particles, especially as opposed to each other, raises an interesting subject for investigation. Both the shock speed V_{sh} and the compression ratio s affect how particle distributions evolve, and often in contradicting (or even self-contradicting) ways. Prior to injection, both properties affect the heating of the SW, while the hardness of shock-accelerated spectra is already shown to depend on the compression ratio.

4.5.1 DSA for different compression sizes and shock speeds

To explore and compare the effects of the shock speed V_{sh} and the compression ratio s , these parameters are varied in three different ways: V_{sh} and s are each varied separately with the other

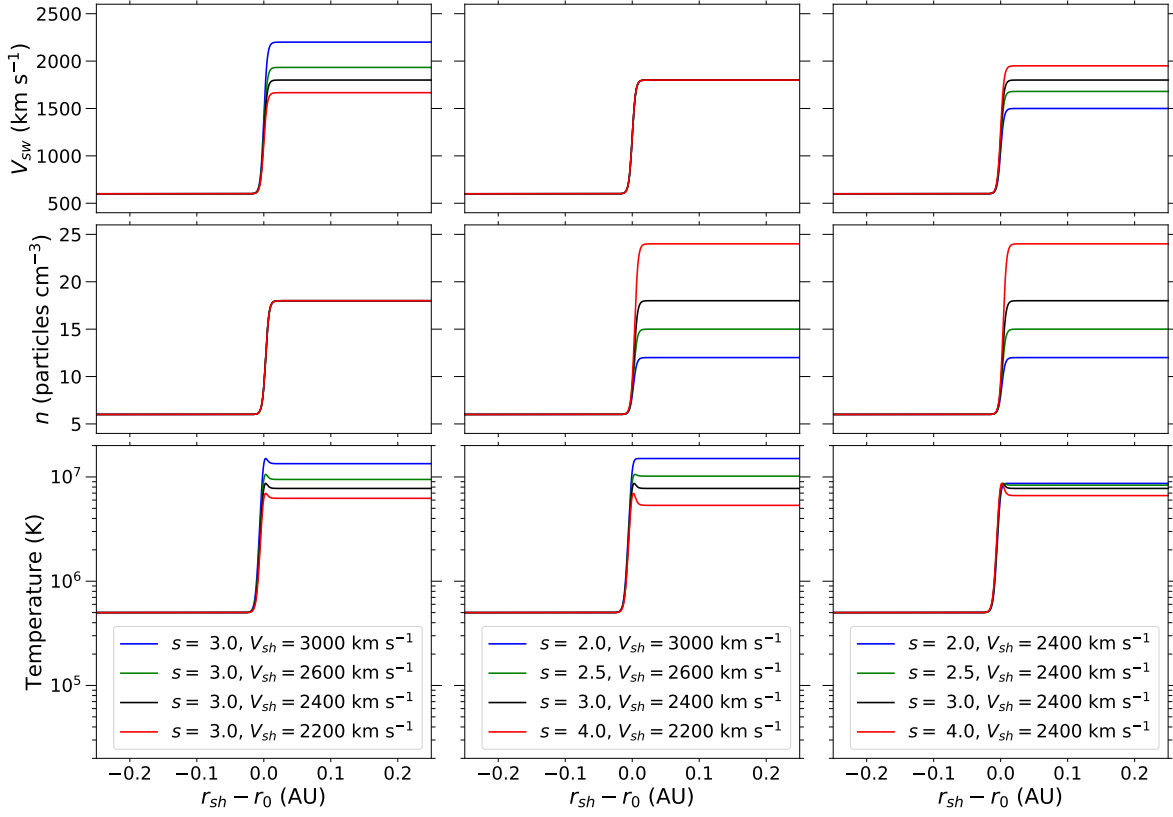


Figure 4.9: Similar to the left-hand side of Figure 4.3, the profiles above are shown for some of the configurations of Table 4.3, where the shock speed V_{sh} and compression ratio s are varied both separately, as shown in the left and right columns, respectively, and together as shown in the middle column. Profiles representing the reference configuration are shown in black.

remaining fixed, and then varied together such that V'_2/V'_1 , the factor by which the fixed-frame flow speed jumps across the shock, remains constant. For ease of reference, these three sets of parameter configurations are shown in Table 4.3, along with the corresponding downstream flow speeds in both the fixed frame and the shock frame, denoted V'_2 and V_2 , respectively.

Varying V_{sh} and s affects the shock transitions of the SW flow speed, number density, and temperature, and thereby also influences how the energy distribution of SW particles changes during the passage of the shock. Each of the aforementioned parameters' shock transitions are shown in Figure 4.9 for the configurations listed in Table 4.3. The fixed-frame flow speed, that is, the flow speed as viewed by an observer stationed at Earth, increases with both V_{sh} and s when each is varied separately. The results, as shown in the top row of frames in Figure 4.9, show larger jumps in flow speed should either V_{sh} or s be increased. As intended, when V_{sh} and s are varied together, the downstream flow speed remains constant in the fixed frame. Hence the factor by which the flow speed increases is the same for these instances. The corresponding shock transitions of the number density and temperature in Figure 4.9 follow from Eqs. 4.14 and 4.16. Figure 4.10 shows how the SW energy distributions change in response to these shock transitions. It appears that the SW energy distribution is heated by comparable amounts for varying shock speeds and strengths. However, j_κ appears marginally more sensitive to changes in temperature, which in turn is affected most appreciably by changes in V_{sh} . Therefore, it can be argued that V_{sh} contributes more towards heating the SW distribution, compared to s ,

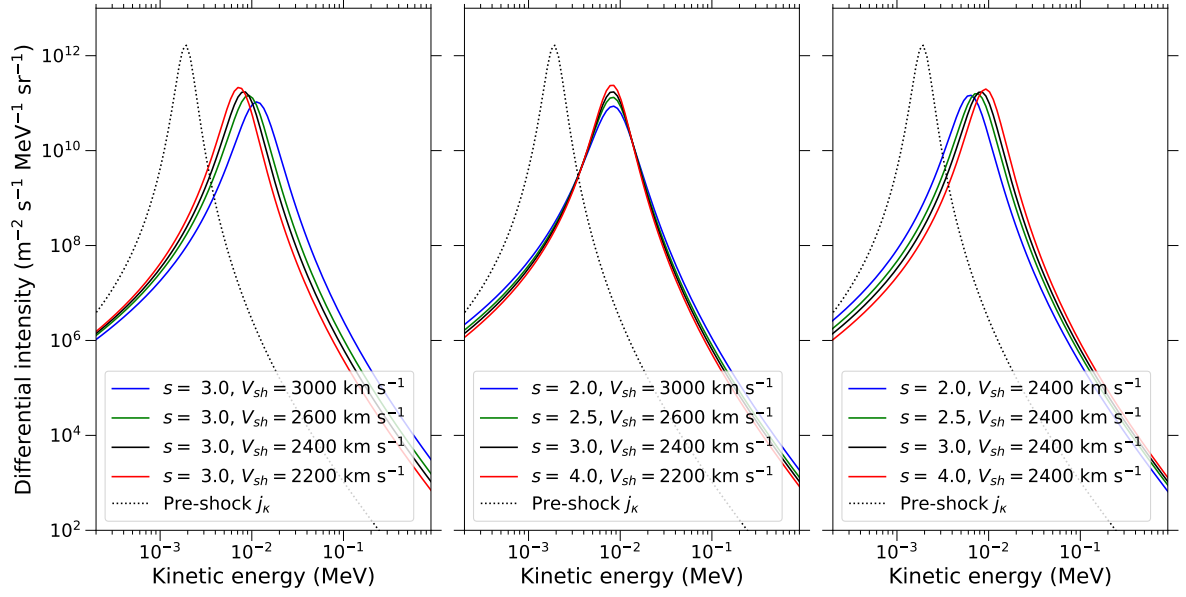


Figure 4.10: The heating of the SW energy distribution at Earth in response to the shock transitions of the plasma parameters in Figure 4.9. Distributions are shown for the same shock speed and compression ratio configurations used in the corresponding columns of Figure 4.9. Dotted lines represent the unperturbed SW energy distributions from before the shock passage.

considering the large shifts in energy and the broadening of j_κ that follows from varying V_{sh} .

The heated SW distributions discussed above essentially serve as input spectra, from which particles are injected into the DSA process at the shock for $E > E_{inj}$. The shock-accelerated spectra obtained by solving the SDEs of Section 4.2.1 for each of the configurations in Table 4.3 are presented in Figure 4.11. The analyses of these spectra are analogous to those of spectra presented in Figure 4.4, and the discussions that follow draw on concepts introduced in Section 4.4. Accordingly, functions are fitted to the SDE solutions and the parameters tabulated for each configuration in Table 4.4. The value of λ_0 is chosen as 0.06 AU throughout this section. With reference to Figure 4.6, this implies the diffusion length scale exceeds the shock width for all considered energies and that the full compression ratio is sampled. It is therefore sufficient to fit the single power-law function of Eq. 4.18 with spectral indices as predicted by DSA.

The shock-accelerated spectra presented in Figure 4.11 share the same general features as those encountered before: a power-law segment extending from near the injection energy up to where it rolls over into an exponential decrease. The following discussion considers how these features change as a result of varying the shock speed V_{sh} and compression ratio s . Firstly, varying V_{sh} , while keeping the compression ratio fixed at $s = 3$ produces spectra shown in the left column of Figure 4.11. These spectra are power-law distributed with a spectral index of -1.25 , as illustrated in the accompanying bottom frame. This is the index expected from DSA for $s = 3$ (see Eq. 4.19). The sizeable differences in the intensities of these three spectra are due, in large part, to the heated SW spectra, which themselves are notably affected by varying V_{sh} . When varying s instead and keeping the shock speed fixed at $V_{sh} = 2400 \text{ km s}^{-1}$, as shown in the right-most column of Figure 4.11, intensities differ mostly due to changes in the power-law indices of shock-accelerated spectra. These indices, shown in the accompanying bottom frame as -2 , -1.25 and -1 , correspond to those expected from Eq. 4.19 for $s = 2, 3$, and 4 ,

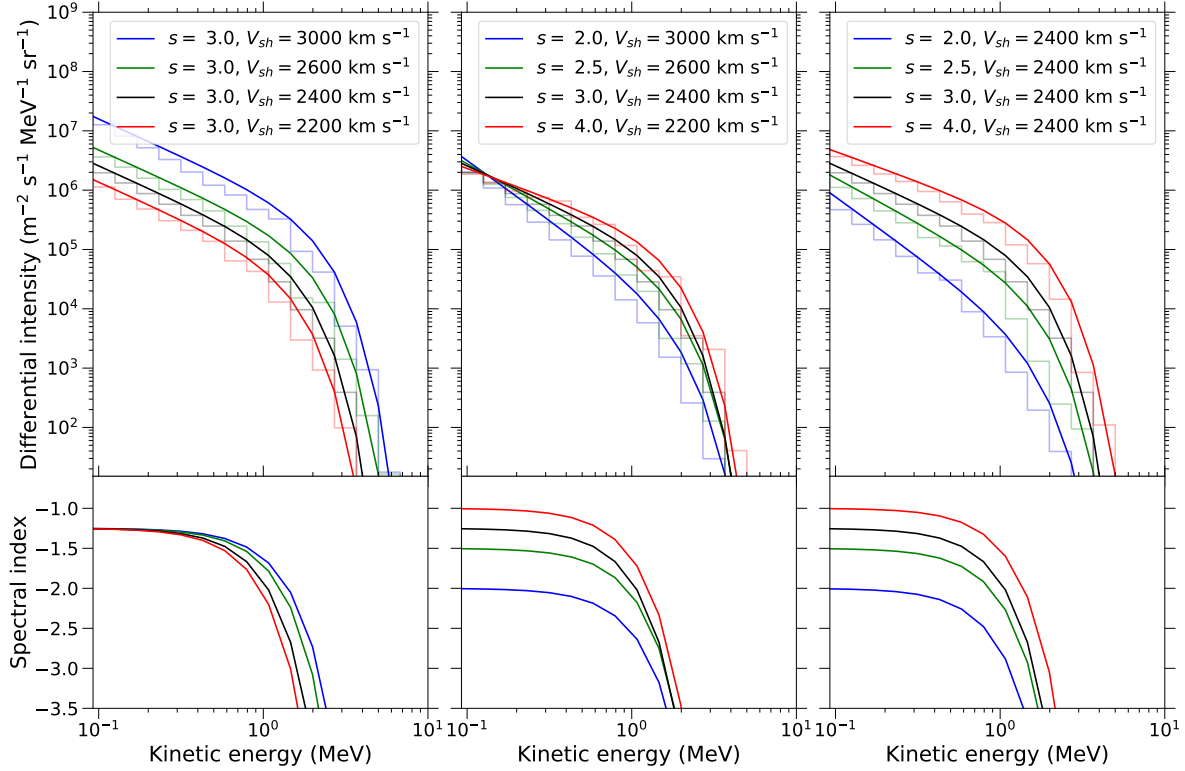


Figure 4.11: Top: Modelled shock-accelerated energy spectra at the Earth at the time of the shock passage for some of the configurations listed in Table 4.4 and with the corresponding SW distributions of Figure 4.10 specified as input spectra. Step-like lines represent SDE solutions, while the smooth solid lines are corresponding fits of Eq. 4.18 using the parameters listed in Table 4.4. Bottom: Corresponding spectral indices for spectra shown above.

respectively.

The middle column of Figure 4.11 illustrates the case where both V_{sh} and s are varied so that $V'_2/V'_1 = 3$. It is worth drawing attention to the fact that the spectral indices displayed by these spectra are not the index associated with $V'_2/V'_1 = 3$, even though this would be the jump factor in the flow speed observed by spacecraft during the passage of the shock. The power-law indices of all shock-accelerated spectra are consistently those associated with s . The observed factor by which flow speeds change across a shock should not be confused with the actual compression ratio, which is the factor by which either the density or the flow speeds in the shock frame change across the shock. This is important when calculating the power-law index of the DSA-predicted spectrum for comparison with an observed energy spectrum.

The spectra shown in the left and right-hand sides of Figure 4.11 extend to higher energies for both faster and stronger shocks, where V_{sh} and s are each varied separately with the other held constant. This trend is also illustrated in Figure 4.12. By contrast, when V_{sh} and s are varied together, as specified in Table 4.3, the spectra in the centre panel of Figure 4.11 extend up to similar energies. This is emphasised in the shaded regions in Figure 4.12, which show that the cut-off energies do not respond appreciably to the changing shock conditions. Similar to Section 4.4.2, the acceleration times corresponding to each of the spectra in Figure 4.11 are calculated and compared to the simulation times, as shown in Figure 4.13. As before, the maximum attainable energies for shock-accelerated spectra are determined predominantly by the shock transit time.

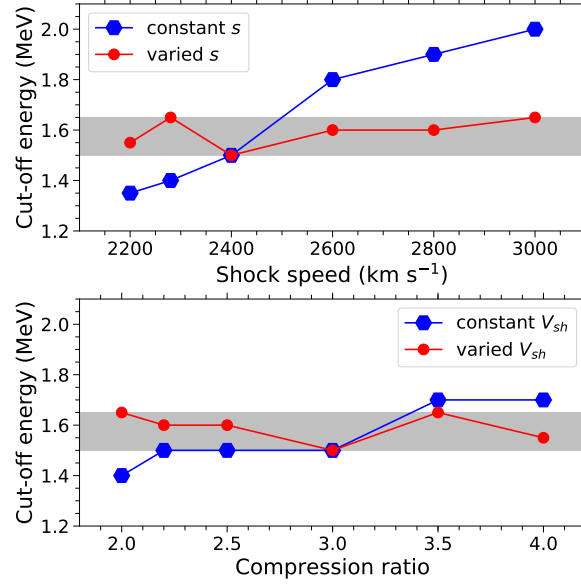


Figure 4.12: Cut-off energies, where spectra roll over into exponential decreases, as functions of shock speed V_{sh} and compression ratio s , for configurations where V_{sh} and s are varied both separately and together as specified in Table 4.4. Shaded regions indicate the comparatively small variations in cut-off energies when the parameters are varied together.

4.5.2 Acceleration efficiency: Strong versus fast shocks

The preceding sections analyse the collated effects of varying V_{sh} and s during the complete acceleration process, including the heating of the SW energy distribution and the subsequent shock acceleration. It can be argued that the shock speed has the largest effect, since varying V_{sh} yields pronounced changes in both the heated SW distributions and in reducing acceleration times, thereby extending spectra to higher energies. On the other hand, the most notable effect of varying s is the changes in the power-law indices displayed by shock-accelerated spectra, which also affects energetic particle intensities considerably.

Implementing the same technique used in Section 4.4.3, particle fluences are calculated using Eq. 4.23. The resulting energy-integrated intensities are shown in the top frames of Figure 4.14 as functions of both V_{sh} and s . To constrain the intensities resulting solely as a result of DSA and not including those of the input spectra, fluences are also calculated for the heated SW distributions (I_{kappa}) and subtracted from those calculated for the shock-accelerated spectra (I_{total}). These two additional sets of energy-integrated intensities, namely I_{kappa} and $I_{\text{DSA}} = I_{\text{total}} - I_{\text{kappa}}$, are also shown in Figure 4.14. Note that I_{kappa} is roughly an order of magnitude smaller than I_{total} on average, with comparably weak dependences on V_{sh} and s . The fluence I_{DSA} therefore closely resembles I_{total} . Considering particle fluences as functions of V_{sh} and s , where each is varied alone, it is apparent that both faster and stronger shocks yield greater numbers of energetic particles, whether considered for $E > E_{inj}$ or for $E > 1$ MeV. Since compression ratios for shocks in the SW do not typically exceed 4, and there is no hard limit on the speed shocks can attain, faster shocks arguably have greater potential as particle accelerators.

It is insightful to consider fluences for the configurations where V_{sh} and s are varied together, since this is essentially comparing the acceleration efficiencies of strong slower-moving shocks

	V_{sh} (km s ⁻¹)	s	$\gamma(s)$	E_{cut} (MeV)
1:	3000	3	-1.25	2.0
	2800	3	-1.25	1.9
	2600	3	-1.25	1.8
	2280	3	-1.25	1.4
	2200	3	-1.25	1.35
2:	2400	2	-2.0	1.4
	2400	2.2	-1.75	1.5
	2400	2.5	-1.5	1.5
	2400	3.5	-1.1	1.7
	2400	4	-1.0	1.7
3:	3000	2	-2.0	1.65
	2800	2.2	-1.75	1.6
	2600	2.5	-1.5	1.6
	2280	3.5	-1.1	1.65
	2200	4	-1.0	1.55
ref:	2400	3	-1.25	1.5

Table 4.4: Parameters used to fit Eq. 4.18 to the solutions of Figure 4.11 and corresponding to the configurations of shock speed V_{sh} and compression ratio s introduced in Table 4.3. Here, $\gamma(s)$ is the spectral index associated with s as given by Eq. 4.19, and E_{cut} is the energy at which spectra roll over into exponential decreases. The last line contains the reference configuration.

against weaker fast-moving shocks. For these cases, fluences remain fairly constant for all combinations of V_{sh} and s for $E > E_{inj}$. However, if only the number of higher-energy particles is considered, where $E > 1$ MeV, the results are more interesting: as function of compression ratio, the fluences increase as shocks become stronger, despite simultaneously becoming slower. As a function of the shock speed, these fluences become smaller for faster shocks for which the accompanying compression ratios are smaller. This implies that strong, slower-moving shocks are able to produce a greater number of energetic particles than weak fast-moving shocks, at least within the parameter ranges considered and for shocks with $V_2'/V_1' = 3$.

4.6 From the solar wind to energetic storm particles

In this section, the development of particles injected from the suprathermal SW into energetic particles associated with ESP events is considered in greater detail. The underlying question of how SW particles can be accelerated to the much higher energies at which ESPs are observed is visually represented in the left panel of Figure 4.15. The intensities observed during the Halloween ESP event of 2003 October 29 are shown as an example of typical energy spectra observed during such events. Note this particular spectrum is reproduced well by the power law associated with $s = 4$ [e.g. Giacalone, 2015].

The acceleration process is initiated with the heating of the SW energy distribution, where the κ -function describing it is allowed to change in response to changes in flow speed, density, and temperature across the shock as shown in Section 4.3.2. The importance of this initial heating cannot be understated. Consider, firstly, a spectrum shock-accelerated from the original, undisturbed SW distribution. It would likely not extend up to the energies of observed ESPs because

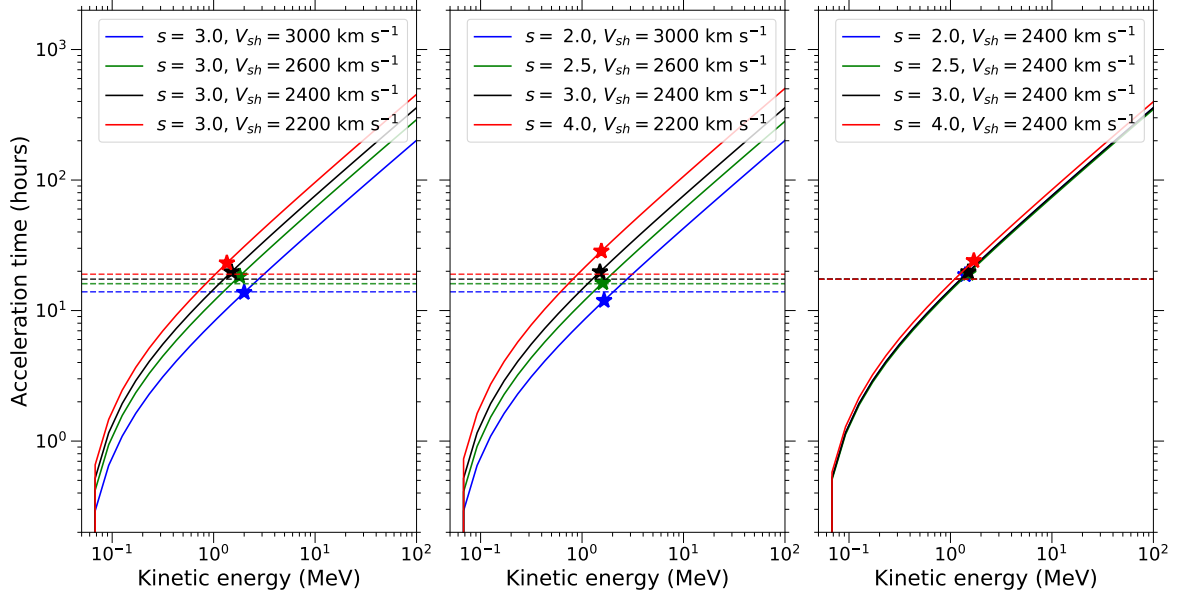


Figure 4.13: Acceleration times, similar to Figure 4.7, for each of the configurations of V_{sh} and s corresponding to the spectra shown in Figure 4.11. Markers indicate the time required to accelerate spectra up to the corresponding cut-off energies (E_{cut}) listed in Table 4.4. The total simulation times (indicated as dashed horizontal lines) correspond to configurations represented in the same color and indicate the travel times of the shock moving at V_{sh} between the Sun and the Earth.

of the limited time available for acceleration. Secondly, assuming the injection threshold for DSA is much larger than thermal energies, the larger intensities associated with the heated SW could allow shock-accelerated intensities to reproduce those of typical ESPs. Indeed, the bottom-left panel of Figure 4.15 illustrates that the heated SW distribution increases intensities of potential DSA seed particles by up to a factor of 10^4 , while increasing suprathermal tail intensities a hundredfold at least. Interestingly, observations suggest that peak fluxes during ESP events display some dependence on CME sheath temperature [Dayeh *et al.*, 2018], while the broadening of SW distributions (which influence eventual intensities of shock-accelerated particles) is predominantly dictated by temperature changes across the shock.

4.6.1 Injection from the heated SW distribution

In the simplest terms, the injection threshold for DSA can be considered to be the minimum energy required for particles to catch up with the shock and make repeated shock crossings. This injection energy can be inferred by matching theoretically expected shock-accelerated spectra with observations [*e.g.* Neergaard-Parker and Zank, 2012]. It can also be estimated using the argument that the particle anisotropy must be small in order for DSA to be valid [Giacalone and Jokipii, 1999; Zank *et al.*, 2006]. For the typical values implemented in this study ($V_1' = 600 \text{ km s}^{-1}$, $s = 3$), injection energies are of the order of a few keV for parallel shocks, for which injection from an unheated Maxwellian seed particle distribution would indeed be possible [Neergaard-Parker and Zank, 2012]. However, for quasi-perpendicular shocks, and in the absence of magnetic field-line wandering, it is estimated that $E_{inj} \gtrsim 0.1 \text{ MeV}$ [see also Li, 2017]. The prior heating of the SW distribution becomes especially useful in this situation. See also the simplified method used by Hu *et al.* [2017] to estimate injection energies.

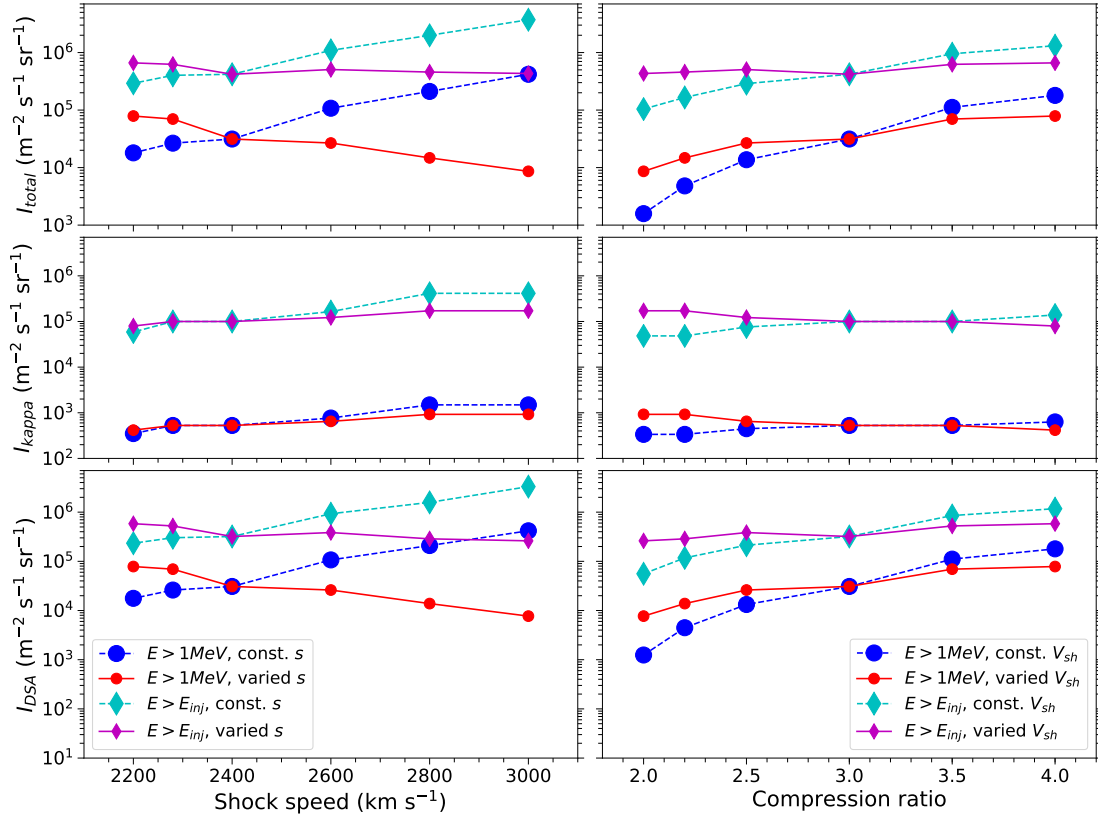


Figure 4.14: The energy-integrated intensities (or fluences) of energetic particles above the injection energy (E_{inj}) and 1 MeV, represented by diamond and dot markers, respectively, as functions of shock speed V_{sh} and compression ratio s . Quantities I_{total} , I_{kappa} , and I_{DSA} represent fluences for shock-accelerated spectra, heated SW distributions and those resulting from DSA alone, where $I_{\text{DSA}} = I_{\text{total}} - I_{\text{kappa}}$. The SW speed V_{sh} and compression ratio s are varied both separately and together for configurations as specified in Table 4.3.

The halo-CME shocks considered in this study are mostly quasi-parallel if a *Parker* [1958] spiral is assumed for the magnetic field. Here, E_{inj} is varied between 10 and 60 keV, spanning an energy domain extending from the thermal peak to the suprathermal tail of the heated SW distribution, and bounded by the aforementioned estimates for parallel and quasi-perpendicular shocks. The effects of these varied injection thresholds on shock-accelerated spectra are shown in the right panel of Figure 4.15. As before, Eq. 4.20 is fitted for each case and the parameters listed in Table 4.5. The reference configuration, as specified in Table 4.3, is used, with $\lambda_0 = 0.06$ AU, $V_{sh} = 2400 \text{ km s}^{-1}$, and $s = 3$. The standard features are visible: the spectra are distributed according to $E^{-1.25}$ as expected for $s = 3$ and roll over exponentially at higher energies. Spectra appear to terminate at similar energies for the injection thresholds considered, as this is presumably governed by the acceleration time.

It can be seen from the right panel of Figure 4.15 that injecting particles from the heated SW distribution yields high intensities in the energy domain typically associated with ESPs. In the case of $E_{inj} = 60 \text{ keV}$, the shock-accelerated intensities are quite similar to those observed for the ESP event included in Figure 4.15 as an example. Should the injection speed be defined as the minimum possible speed a particle needs to stay ahead of the shock, whilst following a Parker field line with a 45° angle ahead of the shock nose, the injection speed can be written as $v_{inj} \sim |V'_1 - V_{sh}| / \cos(45^\circ)$ (cf. Eq. 2.3). For a fast halo-CME shock with $V_{sh} = 2400 \text{ km s}^{-1}$ and

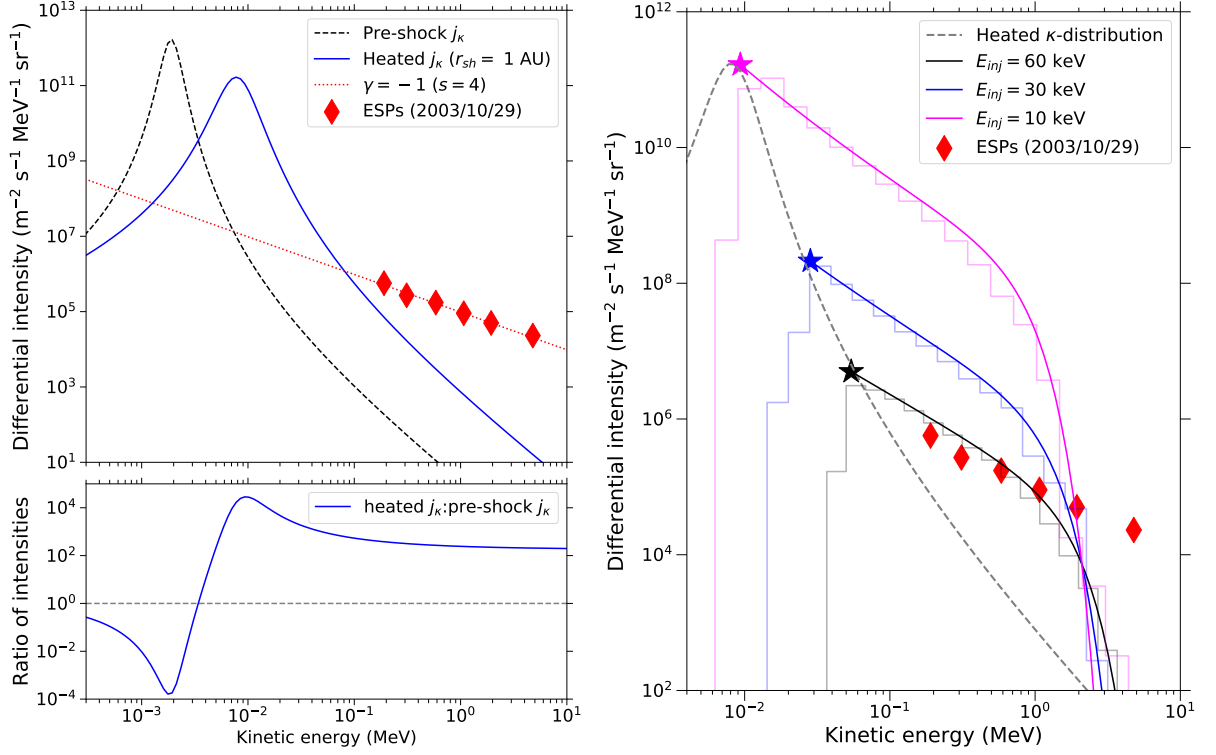


Figure 4.15: Left: The undisturbed and heated SW energy distributions at Earth, with the latter corresponding to the time at which the shock passes the Earth’s position. The ratios of these distributions are shown in the bottom panel. Right: Modelled shock-accelerated spectra at the Earth at the time of the shock passage for different injection energies. Step-like lines represent SDE solutions while the solid lines are fits of Eq. 4.20 with parameters as listed in Table 4.5. The dashed grey line represents the heated SW distribution. Diamond markers represent intensities observed by *ACE*/EPAM LEMS30/120 during an energetic particle event on 2003 October 29, fitted (on the left) with the E^{-1} power law associated with a strong shock of $s = 4$.

E_{inj} (keV)	γ_a	E_{tr} (keV)	E_{cut} (MeV)
10	-2.0	30	0.7
30	-1.8	30	1.0
60	-1.25	-	1.5

Table 4.5: Parameters used to fit Eq. 4.18 to the solutions in the right panel of Figure 4.15 for different injection energies E_{inj} . All quantities are as described for Table 4.2.

a more typical upstream flow speed of 400 km s^{-1} , the injection speed at 1 AU in the upstream flow frame is $v_{\text{inj}} = 2828 \text{ km s}^{-1}$, which corresponds to an injection energy of $E_{\text{inj}} \sim 50 \text{ keV}$. This is reasonably similar to the 60 keV injection energy required to fit the presented observations using the heated κ -distribution as a source.

The presented simulations are not intended to reproduce observations exactly, nor is it posited that the spectrum observed during the presented ESP event is the unambiguous result of particles accelerated from the SW. The aforementioned results do however demonstrate that the prior heating of the SW energy distribution complements the shock acceleration process well and might even be necessary when considering shocks with large injection energies.

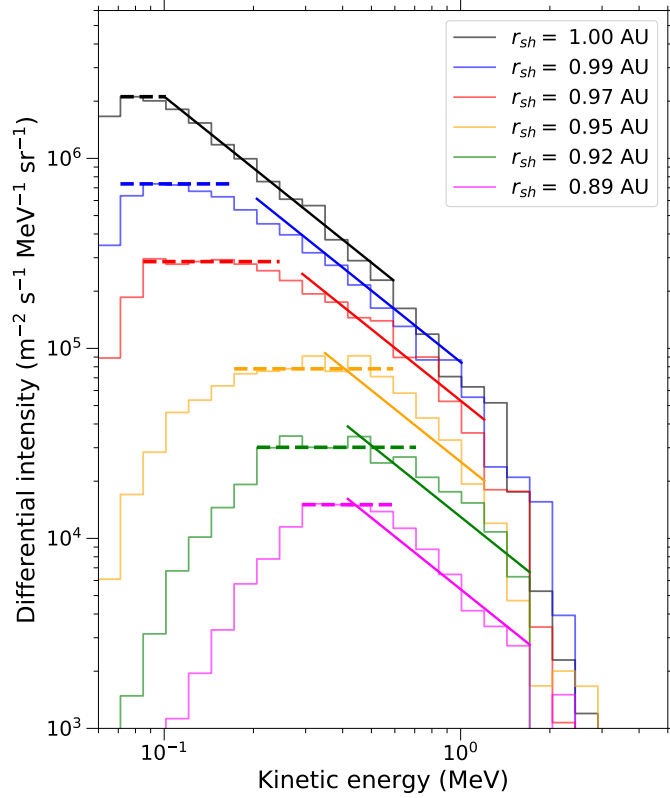


Figure 4.16: Modelled shock-accelerated spectra at the Earth at different times during the approach of the shock. Step-like lines represent SDE solutions, dashed lines indicate flat segments, and the thick solid lines indicate power law segments that are distributed as $E^{-1.25}$ as expected from a shock with $s = 3$.

4.6.2 The evolution of shock-accelerated distributions during the shock passage

Particles of sufficient energy can be injected into the DSA process at any time during a CME shock's passage between the Sun and the Earth. However, ESP events entail the local enhancement of particle intensities as viewed by spacecraft at Earth. The largest enhancement is naturally expected when the shock reaches Earth. Solving the time-backward SDEs for the reference configuration and different starting positions of the shock, the energy spectra and intensity profiles of shock-accelerated particles are simulated for the approach and aftermath of the shock's passage at Earth. These are shown in Figures 4.16 and 4.17, respectively.

The time-evolution of energy spectra during the approach of the shock is considered first. From Figure 4.16, the most recognizable aspect is of course the power-law form of the spectrum at the time of the shock's arrival at Earth, where $r_{sh} = 1$ AU, followed by a cut-off at higher energies. However, this spectrum appears to be notably different when the shock is just 0.01 AU away, which for $V_{sh} = 2400 \text{ km s}^{-1}$ is a few minutes before its arrival at Earth. The differences, which become starker for larger distances between the shock and the Earth, include lower overall intensities and a downturn in the spectrum at low energies. The progressively lower intensities follow both because the particle source at the shock is further away, and because the shock-accelerated particles are modulated while they propagate ahead of the shock toward Earth. This becomes more evident when the shock is far from the Earth.

A particularly interesting feature in Figure 4.16 is the flattening of spectra during the approach

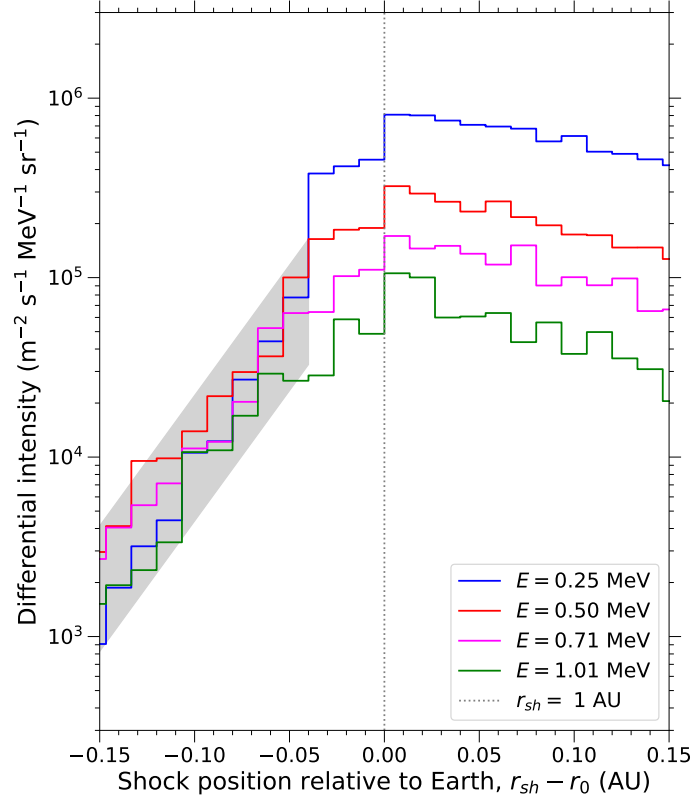


Figure 4.17: Profiles of energetic particle intensities at different energies as viewed by an observer at Earth during the passage of the shock. The vertical dotted line represents the moment of the shock's arrival at Earth. The shaded region accentuates where energy spectra are approximately flat.

of the shock. Similar flattening has recently been reported in observations of proton spectra between 50 keV and 1 MeV prior to the passage of an interplanetary shock at Earth [Lario *et al.*, 2018]. It is conceivable that this is the result of the competing effects of shock acceleration and modulating processes. Shock acceleration tends to distribute particles according to E^{γ_s} , where $\gamma_s = -1.25$ for $s = 3$ according to Eq. 4.19. Therefore, when the shock is nearer to Earth, these shock-accelerated features dominate, whereas particles transported from the shock while it is still further upwind have been modulated to a greater extent. Where these effects balance, the spectrum flattens. There are two modulation processes included in the TPE that may account for this. Firstly, consider that diffusion is assumed to be rigidity dependent in Eq. 4.3, implying that low-energy particles, which have smaller MFPs, will be modulated more than higher-energy particles. This offers the simplest explanation for the low-energy downturns. However, steep spectra with positive power-law indices at lower energies are also known spectral characteristics of adiabatic energy losses [e.g. Moraal and Potgieter, 1982; Strauss *et al.*, 2011]. As a result of progressively stronger modulation, Figure 4.16 shows the flattened segments narrow and move to higher energies for larger distances between the shock and the Earth.

Figure 4.17 shows intensity profiles similar to how the observations of Lario *et al.* [2018] are presented. The flat energy spectra can be discerned from the coinciding intensity profiles of 0.25 to 1 MeV particles. This energy range can be broadened in the simulations by specifying a lower injection energy or assuming stronger shocks for which the shock-accelerated spectrum will be less steep. These flat segments are visible for shock positions up to at least 0.15 AU away from the Earth, that is, for nearly three hours prior to arrival. Note that the shock speed

of 2400 km s^{-1} implemented in these simulations is very fast. If a more typical shock speed of *e.g.* 1000 km s^{-1} [*e.g.* *Mäkelä et al.*, 2011] is assumed, this effect would be visible for a longer time prior to the shock's arrival at Earth. The intensity profiles shown in Figure 4.17 largely resemble those of typical ESP events: a large onset of particle intensities over a relatively short time is visible before the arrival of the shock, followed by a more gradual decline of intensities after it has passed. See also the observations of *Lario et al.* [2019] concerning the evolution of suprathermal proton intensities during shock passages at 1 AU.

Note that the peaks of the simulated profiles, corresponding to the arrival of the interplanetary shock at Earth, are not as sharp as observed intensities tend to show. These peaks are often associated with large anisotropies [*e.g.* *Lario et al.*, 2005a], which can be more appropriately modelled using focused transport models [*Zuo et al.*, 2011; *le Roux and Webb*, 2012]. The TPE in this study is solved for an omni-directional distribution function (as discussed in Section 3.2) and describes only the near-isotropic particle component.

4.6.3 Seed-particle energies and initial positions

It only remains to be investigated where and from which energies SW particles contributing to any given observational point are accelerated. To do this, the binning technique discussed in Section 4.2.1 is implemented. Firstly, pseudo particles are traced time-backwards from the observational point $(r_{\text{obs}}, E_{\text{obs}}) = (1 \text{ AU}, 1 \text{ MeV})$, whereafter the average particle amplitudes are calculated for each (r, E) -bin at $t' = 0$. As before, the simulation is run for the reference parameters listed in Table 4.3. The result is shown as a colour-scaled plot in Figure 4.18.

This plot essentially maps the relative contributions of particles from different initial positions and energies to the intensities of 1 MeV particles at Earth's position at the time of the shock's passage. As such, they provide a great deal of insight into the probable original energies and locations of seed particles. Figure 4.18 shows the unperturbed distribution (that is, before the departure of the shock from near to the Sun) of SW particles that would eventually contribute to 1 MeV intensities at Earth. It is illustrated that the largest contributions are from particles initially located upwind from Earth and accelerated from energies ranging from tens to a few hundred keV. The lower limit of this range corresponds to the 60 keV injection energy implemented in this study. The contributions of particles either cooled to 1 MeV from higher energies or convected to Earth without incurring energy changes are minuscule by comparison. The much larger relative contribution of particles accelerated to E_{obs} from lower energies illustrates that DSA at the travelling interplanetary shock is the chief contributor to intensities during the simulated ESP event.

Note that, during the shock transit, the distribution of contributing particles will move closer to the observational point, following the shock front until, at the time of the shock's arrival at Earth, only that point will be populated on the plot with a value of unity. See also the simulation (on the online version) of *Prinsloo et al.* [2019] showing the evolution of the plot in Figure 4.18 as the shock progresses toward Earth.

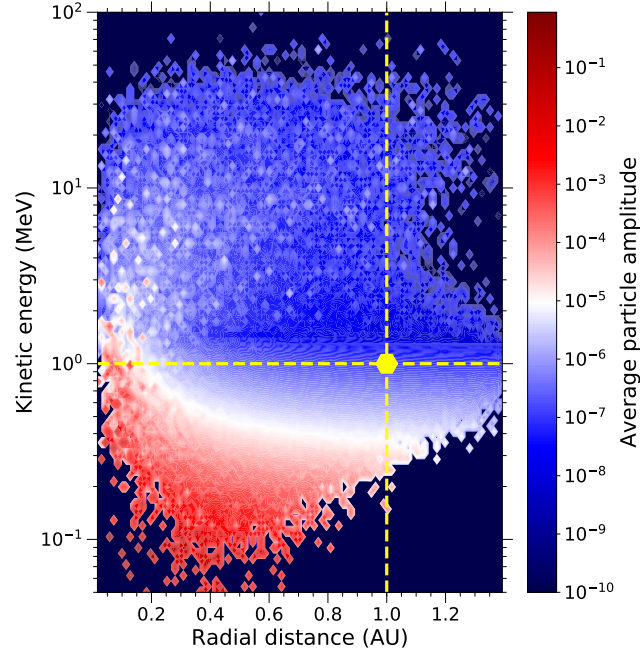


Figure 4.18: Initial radial and kinetic energy distribution of SW particles contributing to 1 MeV intensities at Earth during an ESP event. The color scale indicates the average particle amplitudes at each (r, E) -point, where the maximum amplitude has been normalised to unity. The observational point, from where pseudo-particle trajectories are traced in a time-backwards fashion, is shown as a marker at the intersection of vertical and horizontal dashed lines indicating Earth's position and 1 MeV, respectively.

4.7 Summary and conclusions

In this chapter, the acceleration of SW particles at halo CME-driven interplanetary shocks is investigated. The thermal and suprathermal components of the SW velocity (or equivalent energy) distributions are collectively described using κ -functions. The SW distributions are transformed in response to simulated shock transitions in the plasma properties on which they depend, such as the flow speed, number density, and temperature. These transformed (or heated) distributions are consequently specified as source spectra, from which particles with sufficient energy can be injected into the DSA process at the shock. To model this acceleration process, SDEs equivalent to the Parker TPE are solved in a time-backwards fashion. Using the combined approach of the pre-injection heating of the SW distribution and DSA, simulations reveal a number of noteworthy results with regards to the particle acceleration at interplanetary shocks, and particularly of SW particles.

The simulations are shown to produce the classical spectral features of DSA. However, in cases where diffusion length scales are small relative to the shock width, shock-accelerated spectra do not display the spectral indices associated with the full compression ratio. Such situations may arise in the case of high levels of magnetic turbulence, which can decrease diffusion length scales, or in the case of broader compressions in the SW [e.g. Giacalone et al., 2002]. At any rate, the softer power-law distributions that are attained as a result notably reduce the overall intensities of shock-accelerated particles. Furthermore, it is shown that the highest attainable energies of shock-accelerated spectra are limited by the transit time of the shock. Reduced diffusion length scales may serve to better confine particles near the shock, thereby allowing

spectra to be accelerated to higher energies within the available time. Intensities of higher-energy particles ($E > 1$ MeV) are shown to be particularly sensitive to this time limit.

The dependence of DSA on shock properties such as speed and compression ratio is also investigated. Fast shocks contribute appreciably to the heating of the SW distribution. While fast-moving shocks have shorter associated transit times, allowing less time for particle acceleration, larger shock speeds have a net positive effect on particle acceleration. Through their contribution to larger flow speeds they reduce diffusion length scales, improving particle confinement at the shock. They also reduce the time required for acceleration. Since larger shock speeds imply larger differences of flow speeds across the shock, a particle scattered across it experiences a larger mean energy gain per crossing [Drury, 1983; Kong *et al.*, 2019]. This can also be thought of as scattering centres converging on the shock at higher rates for fast shocks.

The compression ratio, as measure of shock strength, also affects the magnitude of flow speed transitions across the shock, providing the actual factor by which both the shock-frame flow speed and number density change across the shock. In particular, larger compression ratios increase intensities of the SW distribution across the shock, since the κ -function is normalised to the number density. While it has a more modest effect on acceleration times than the shock speed, its effect on overall particle intensities is significant, since the spectral indices of the shock-accelerated spectra depend directly on the compression ratio. When strong and fast shocks are compared as particle accelerators, it is found that strong slower-moving shocks produce larger numbers of energetic particles than weak fast-moving shocks. The compression ratio, being directly associated with the steepness of accelerated energy distributions, is therefore identified to be the greater limiting factor of these two shock properties.

With regards to simulating ESP events, the prior heating of the SW distribution during the shock passage is found to complement the DSA process well: it provides greater intensities of potential seed particles for DSA, especially where large injection energies are considered, and allows shock-accelerated spectra to achieve large enough intensities at sufficiently high energies to reproduce typical ESP events. This result is consistent with observations reporting larger peak particle fluxes during ESP events for warmer CME sheath temperatures [Dayeh *et al.*, 2018]. Furthermore, simulations of shock-accelerated intensities at Earth reveal significant flattening of spectra forming ahead of the shock during its approach. This is found to result from the modulation of shock-accelerated particles while propagating toward Earth ahead of the shock, whether owing to rigidity-dependent diffusion or by means of adiabatic cooling in the expanding SW. These provide potential explanations for similar features recently reported in observations [Lario *et al.*, 2018].

Finally, taking advantage of the time-backward tracing of phase-space density elements, with their flux contributions weighted according to particle amplitude, it is revealed that most SW particles contributing to intensities during a simulated ESP event are transported to Earth from upwind and are accelerated from energies ranging from tens to a few hundreds of keV. Due to the larger fraction of particles accelerated to 1 MeV from lower energies, it can be concluded that DSA is indeed a chief contributor to intensities at Earth during ESP events. It is demonstrated in this chapter that the SDE approach, while shown in Appendix B.1 to yield comparable results to finite-difference methods, can be used to reveal unique physical insights

with regards to particle transport and acceleration at interplanetary shocks. Along with its computational advantages, the SDE model introduced here can be expanded to include more spatial dimensions, providing a means to explore more complicated shock geometries. This is explored further in following chapters.

It is ultimately concluded that with the combination of prior heating and shock acceleration, energetic particles can be accelerated from the suprathermal SW at interplanetary shocks, and that these particles may make appreciable contributions to intensities during observed ESP events. Also, the reproduction of the observed flat energy spectra ahead of shock passages [*Lario et al.*, 2018], resulting from the competing processes of DSA and particle modulation, illustrates the advantage of studying particle acceleration in association with transport processes.

Chapter 5

Two-dimensional transport of shock-accelerated particles

5.1 Introduction

In Chapter 4 spherical symmetry was assumed to study particle acceleration at halo-CME shocks. Whereas ESP events are most often associated with the passage of these very broad shocks, CMEs do vary in longitudinal width, ranging from $\sim 50^\circ$ to 300° [e.g. *Mäkelä et al.*, 2011]. The description of particle acceleration by shocks with finite longitudinal widths and the subsequent transport of these particles to observers must be described in at least two spatial dimensions. Particle diffusion in this configuration is described relative to magnetic field lines as opposed to the radial direction alone. Indeed, the geometry of magnetic field lines is identified as an important factor organizing the longitudinal distributions of shock-accelerated particle intensities during SEP events [e.g. *Cane et al.*, 1988].

This chapter introduces a simple CME-shock geometry as an expansion of the spherical model used in the previous chapter to two spatial dimensions. It is once again assumed that particles are accelerated from the heated SW distribution. Assuming furthermore that transport is limited to the heliographic equatorial plane, the effects that shocks of various longitudinal extents have on the intensities registered by an observer in the path of the shock are investigated. The relative importance of diffusion parallel and perpendicular to magnetic field lines are also investigated for observers both in and outside of the shock path.

Note that it is by no means the purpose of this chapter to present realistic reproductions of CME properties. Instead, concepts pertinent to the next chapter (concerning CIR-related shocks) are introduced within the familiar context of CME-driven shocks as explored in Chapter 4.

5.2 An adapted model for two-dimensional applications

To simulate the transport of particles in the equatorial (r, ϕ) -plane, the *Parker* [1958] spiral is used to describe the magnetic field. This field has no polar component. Therefore $\zeta = 0$, from

which the simplification of the diffusion tensor (Eq. 3.22) follows as

$$\begin{aligned}
 \kappa_{rr} &= \kappa_{||} \cos^2 \psi + \kappa_{\perp r} \sin^2 \psi \\
 \kappa_{\phi r} &= \kappa_{r\phi} = (\kappa_{\perp r} - \kappa_{||}) \sin \psi \cos \psi \\
 \kappa_{\phi\phi} &= \kappa_{||} \sin^2 \psi + \kappa_{\perp r} \cos^2 \psi \\
 \kappa_{\theta\theta} &= \kappa_{\perp\theta} \\
 \kappa_{\theta r} &= \kappa_{r\theta} = \kappa_{\theta\phi} = \kappa_{\phi\theta} = 0,
 \end{aligned} \tag{5.1}$$

where $\psi = \tan^{-1}(\Omega(r - r_{\min}) \sin \theta / V_{sw})$ describes the winding angle between the average magnetic field and the radial direction, with $r_{\min} = 5r_{\odot}$. It is furthermore assumed that particles are transported across the equatorial plane in a symmetric fashion. Therefore, neglecting changes in the θ -coordinate, Eq. 3.23 reduces to

$$\begin{aligned}
 \frac{\partial f}{\partial t'} &= \left(\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \kappa_{rr}) + \frac{1}{r \sin \theta} \frac{\partial \kappa_{\phi r}}{\partial \phi} - V'_{sw} \right) \frac{\partial f}{\partial r} \\
 &+ \left(\frac{1}{r^2 \sin \theta} \frac{\partial}{\partial r} (r \kappa_{r\phi}) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial \kappa_{\phi\phi}}{\partial \phi} + \Omega_{\odot} \right) \frac{\partial f}{\partial \phi} \\
 &+ \kappa_{rr} \frac{\partial^2 f}{\partial r^2} + \frac{\kappa_{\phi\phi}}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2} + \frac{2\kappa_{r\phi}}{r \sin \theta} \frac{\partial^2 f}{\partial r \partial \phi} \\
 &+ \frac{1}{3r^2} \frac{d}{dr} (r^2 V'_{sw}) \xi(E) E \frac{\partial f}{\partial E} + Q.
 \end{aligned} \tag{5.2}$$

This TPE for two spatial dimensions is written in the form of the time-backwards Kolmogorov equation, from which the SDEs for coordinates r , ϕ , and E are written as

$$\begin{aligned}
 dr &= \mu_r dt + \sigma_{rr} dW_r + \sigma_{r\phi} dW_{\phi} \\
 d\phi &= \mu_{\phi} dt + \sigma_{\phi\phi} dW_{\phi} \\
 dE &= \mu_E dt,
 \end{aligned} \tag{5.3}$$

with the coefficients given by

$$\begin{aligned}
 \mu_r &= \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \kappa_{rr}) + \frac{1}{r \sin \theta} \frac{\partial \kappa_{\phi r}}{\partial \phi} - V'_{sw} \\
 \mu_{\phi} &= \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial r} (r \kappa_{r\phi}) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial \kappa_{\phi\phi}}{\partial \phi} + \Omega_{\odot} \\
 \mu_E &= \frac{1}{3r^2} \frac{\partial}{\partial r} (r^2 V'_{sw}) E \xi(E),
 \end{aligned} \tag{5.4}$$

and

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{rr} & \sigma_{r\phi} \\ \sigma_{\phi r} & \sigma_{\phi\phi} \end{bmatrix} = \begin{bmatrix} \sqrt{\frac{2(\kappa_{rr}\kappa_{\phi\phi} - \kappa_{r\phi}^2)}{\kappa_{\phi\phi}}} & \frac{\sqrt{2}\kappa_{r\phi}}{\sqrt{\kappa_{\phi\phi}}} \\ 0 & \frac{\sqrt{2}\kappa_{\phi\phi}}{r \sin \theta} \end{bmatrix}, \tag{5.5}$$

where all quantities are as defined in Sections 3.3 and 3.4. Note furthermore that no additional boundary conditions to those defined in Section 4.2.1 are applied to the coordinates. Once again, the SDEs are solved in a time-backwards manner, starting when the shock is at the

observational point and continued until it reaches the Sun. Similar to Eq. 4.10, the time is variably incremented at each iteration according to which radial transport process (represented in this case by μ_r , σ_{rr} , and $\sigma_{r\phi}$) is dominant.

In contrast to the spherical model of Section 4.2, it is necessary to specify the field-aligned diffusion coefficients in terms of which κ_{rr} , $\kappa_{r\phi}$ and $\kappa_{\phi\phi}$ are defined in Eq. 5.1. Previously, it was assumed that diffusion parallel to field lines dominates, and hence that the rigidity dependence of κ_{rr} reflected that of $\kappa_{||}$, defined by $R^{1/3}$ as predicted by quasi-linear theory [Jokipii, 1966] for a Kolmogorov turbulence power spectrum. This description of $\kappa_{||}$ is also used in this chapter. For perpendicular diffusion, $\kappa_{\perp r}$ is described to have a weak rigidity dependence and to be a few percent of the magnitude of $\kappa_{||}$ [Jokipii et al., 1995; Giacalone and Jokipii, 1999; Burger et al., 2000; Ferreira et al., 2001], that is,

$$\kappa_{\perp r} = \kappa_{\perp,0} \left(\frac{R_0}{R} \right)^{-1/3} \kappa_{||}, \quad (5.6)$$

where $R_0 \approx 1.7$ GV (or $E_0 = 1$ GeV) and $\kappa_{\perp,0} = 0.02$. The rigidity profile described by $\kappa_{\perp r}$ is similar to the Palmer [1982] consensus [see also Bieber et al., 2004, for an alternative description]. As in Section 4.2, the MFP for 1 GeV protons at Earth is chosen such that $\lambda_{rr} \sim 0.06$ AU to correspond with the lower limit of those reported for diffusive SEP events at $r < 1$ AU by Kallenrode et al. [1992]. Furthermore, the same source function (Eq. 4.11) is employed as before, with the description of the κ -function and the SW properties on which it depends as discussed in Section 4.3. However, the shock is specified for a finite longitudinal extent as discussed in the next section.

5.3 A simple 2D CME shock geometry

To simulate a 2D CME-driven shock of finite extent in heliographic longitude, a simple illustrative model is employed where the compression ratio is specified with an azimuthal dependence. By means of Eq. 4.12, this dependence is carried through to the SW properties, and ultimately the SW source distribution, simulating shocked conditions for all quantities within the ϕ -interval for which the shock is defined, but ambient conditions elsewhere.

To this end, the longitudinally dependent compression ratio is specified as

$$s(\phi) = 1 + (s_* - 1) H(\phi_2 - \phi) H(\phi - \phi_1), \quad (5.7)$$

where s_* is the compression ratio equivalent to the jump in density or shock-frame flow speeds across the shock (previously denoted as s), and H is the Heaviside function. The angles ϕ_1 and ϕ_2 are the boundaries of the shock in ϕ , specified such that $\phi_2 > \phi_1$. This yields the following arrangement of compression ratios in ϕ :

$$s(\phi) = \begin{cases} 1 & \phi > \phi_2 \\ s_* & \phi_1 < \phi < \phi_2 \\ 1 & \phi < \phi_1 \end{cases} \quad (5.8)$$

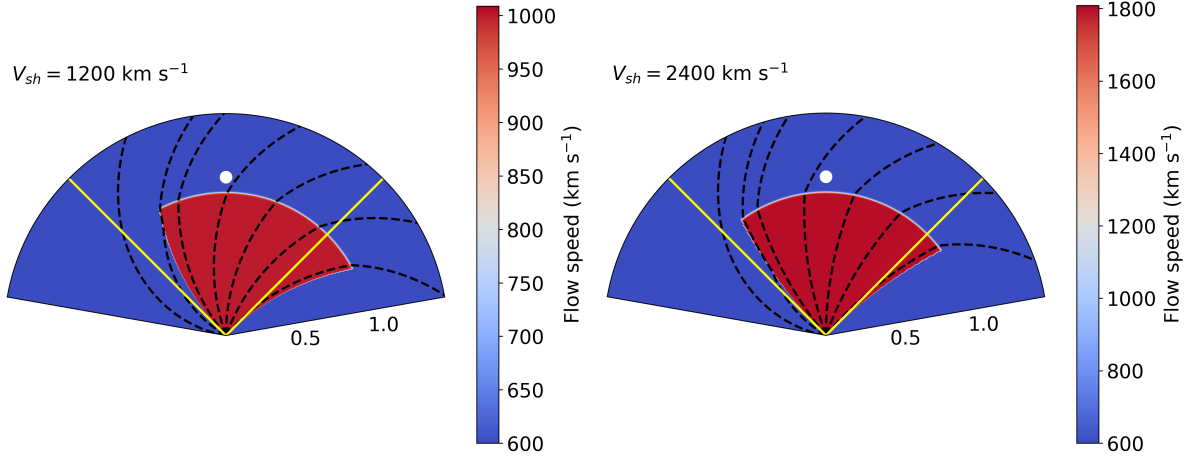


Figure 5.1: Flow speeds associated with the passage of CME-driven shocks, with compression ratios as described by Eq. 5.7, for shock speeds of $V_{sh} = 1200$ and 2400 km s^{-1} in the heliographic equatorial plane and corotating frame. The yellow lines indicate the longitudinal boundaries of the shock in the inertial frame (not rotating with the Sun) at $\phi_1 = 45^\circ$ and $\phi_2 = 135^\circ$. Dashed black lines are equatorial projections of magnetic field lines.

Suppose the shock extends 90° in longitude at its departure from the Sun, with $\phi_1 = 45^\circ$ and $\phi_2 = 135^\circ$. To depict the corresponding flow speeds (calculated from Eq. 4.12) in the frame of an observer corotating with the Sun, the values of ϕ_1 and ϕ_2 must be adapted according to $\phi_\iota = \phi_{\iota,0} - r\Omega_\odot/V_{sh}$, with $\iota \in \{1, 2\}$. The resultant flow speeds are shown in Figure 5.1 for $V_{sh} = 1200$ and 2400 km s^{-1} . In this corotating frame, the CME appears to be dragged out in the opposite direction to the Sun's own rotation, because the Sun is rotating away from the direction of the CME's initial release. The tangential (linear) speed associated with this rotation increases with radial distance as $r\Omega_\odot$ becomes larger compared to V_{sh} . Note that this clockwise drag of the CME is less pronounced for the larger shock speed, because less rotation occurs in the shorter time associated with a faster shock transit. Since the following applications assume $V_{sh} = 2400 \text{ km s}^{-1}$, the relatively small $r\Omega_\odot/V_{sh}$ -term is neglected, and the shock is approximated to advance between constant boundaries in ϕ .

By means of the dependence of the SW flow speed, number density, and temperature on the shock compression ratio (as discussed in Section 4.3.1), the longitudinal dependence of Eq. 5.8 is carried through to the SW distribution as represented by the κ -function. The resultant spatial dependence of the intensities of 40 keV SW particles in the heliographic equatorial plane is shown as a surface plot in Figure 5.2. As this plot shows, downstream of the shock, between $\phi_1 = 45^\circ$ and $\phi_2 = 135^\circ$, suprathermal intensities would increase from the unperturbed SW distribution. This serves to increase the intensities of particles at energies exceeding the injection threshold for DSA ($E \gtrsim 40 \text{ keV}$), although only for a finite region in the ϕ -coordinate as opposed to the heated distributions in Chapter 4, which depend only on r .

Note that Figure 5.1 also shows the associated projections of magnetic field lines onto the heliographic equatorial plane as derived from $d\vec{\ell} \times \vec{B} = 0$, where $d\vec{\ell}$ is the infinitesimal length element in polar coordinates and $\vec{B}$ is the Parker [1958] magnetic field. Across fast-mode shocks such as those typically associated with CMEs, the tangential component of the magnetic field should increase from its upstream value. However, in Figure 5.1, the magnetic field lines are instead less tightly wound in the high-speed flow region trailing the shock front. This follows because

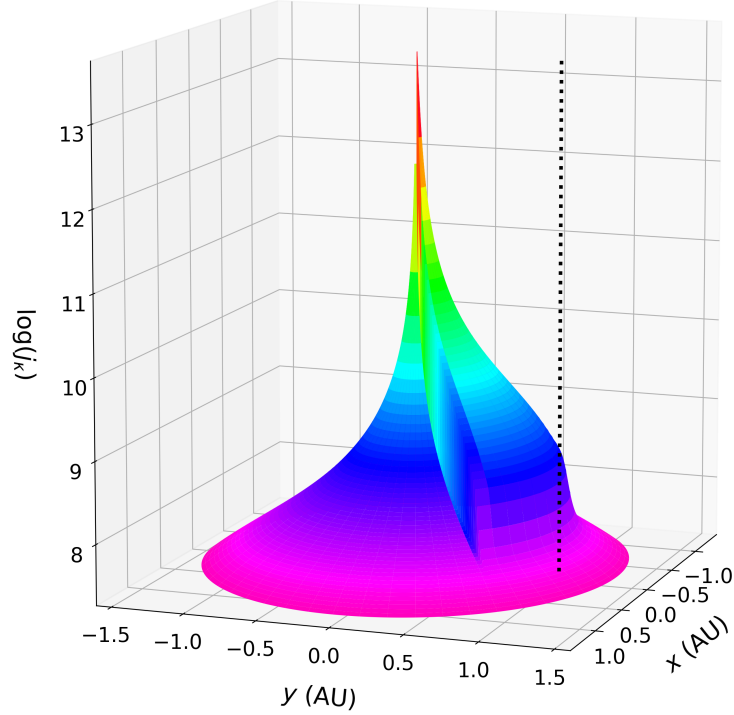


Figure 5.2: Spatial distribution of 40 keV SW particles for the longitudinal dependence of the compression ratio given by Eq. 5.8 for $\phi_1 = 45^\circ$ and $\phi_2 = 135^\circ$, and calculated for the reference parameters listed in Table 4.1. Intensities are expressed in terms of their common logarithms (e.g. $9 \equiv 10^9$), while the vertical line marks the position of an observer at 1 AU and $\phi_{\text{obs}} = 90^\circ$.

the frozen-in magnetic field is convected outward with the SW according to $B \propto 1/V'_{sw}$, and because Eq. 4.12 describes a simple flow speed transition with no turbulent CME sheath region [e.g. Kilpua et al., 2017]. Note that since accelerated particles are expected to be transported to the observer ahead of the shock, and hence predominantly in the upstream medium (see Section 5.5), this description is sufficient for the purposes of this chapter. However, more realistic large-scale reproductions of CMEs and their magnetic properties can be achieved using MHD simulations [e.g. Hu et al., 2017; Scolini et al., 2019].

5.4 Correction for a divergence-free magnetic field

When applying flow speed configurations that are not spherically symmetrical, the magnetic field must, of course, remain divergence-free. For the standard Parker [1958] field, given by $\vec{B} = B_r \hat{e}_r + B_r \tan \psi \hat{e}_\phi$, where $B_r = B_0(r_0/r)^2$ and $\tan \psi = \Omega(r - r_{\min}) \sin \theta / V'_{sw}$, the magnetic field divergence is not zero if the radial flow speed V'_{sw} varies with ϕ . This follows because

$$\frac{\partial B_\phi}{\partial \phi} = \frac{\partial}{\partial \phi} (B_r \tan \psi) = -B_r \frac{\Omega(r - r_{\min}) \sin \theta}{V'^2_{sw}} \frac{\partial V'_{sw}}{\partial \phi} \neq 0, \quad (5.9)$$

if $\partial V'_{sw} / \partial \phi \neq 0$. For the flow speed transition described by Eq. 4.12, it follows that

$$\frac{\partial V'_{sw}}{\partial \phi} = \frac{V_{sh} - V'_1}{2s^2} \left(1 - \tanh \left(\frac{r - r_{sh}}{L} \right) \right) \frac{\partial s}{\partial \phi}, \quad (5.10)$$

if only the compression ratio is assumed to vary with ϕ . It then follows from Eq. 5.7 that

$$\frac{\partial s}{\partial \phi} = (s_* - 1) (H(\phi_2 - \phi) \delta(\phi - \phi_1) + H(\phi - \phi_1) \delta(\phi_2 - \phi)), \quad (5.11)$$

where δ is the Dirac delta function and the Heaviside functions are assumed to be right-continuous, *i.e.* $H(0) = 1$. Note that Eq. 5.11 evaluates to $\partial s / \partial \phi = s_* - 1$ at ϕ_1 and ϕ_2 , but is zero elsewhere. These non-zero values of $\partial s / \partial \phi$ imply that at ϕ_1 and ϕ_2 the magnetic field is not divergence-free.

To address this, a modification is derived to ensure a divergence-free magnetic field for when $\partial V'_{sw} / \partial \phi \neq 0$. Note that, should a B_θ component be included, it follows from $\nabla \cdot \vec{B} = 0$ that

$$\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 B_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (B_\theta \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial B_\phi}{\partial \phi} = 0,$$

where the first term equals zero for $B_r = B_0(r_0/r)^2$. From this and Eq. 5.9 it follows that

$$\frac{\partial}{\partial \theta} (B_\theta \sin \theta) = B_r \frac{\Omega(r - r_{\min}) \sin \theta}{V'^2_{sw}} \frac{\partial V'_{sw}}{\partial \phi}. \quad (5.12)$$

Since the flow speed is assumed not to vary with θ , the above expression is straightforwardly integrated to yield

$$B_\theta \sin \theta = B_r \frac{\Omega(r - r_{\min})}{V'^2_{sw}} \frac{\partial V'_{sw}}{\partial \phi} (C^* - \cos \theta), \quad (5.13)$$

where the integration constant is calculated as $C^* = 1$ by noting that $B_\theta \sin \theta = 0$ at $\theta = 0^\circ$. The modification ensuring a divergence-free magnetic field, represented by B_θ , is therefore given as

$$B_\theta = B_r \frac{\Omega(r - r_{\min})}{V'^2_{sw}} \frac{\partial V'_{sw}}{\partial \phi} \frac{1 - \cos \theta}{\sin \theta}, \quad (5.14)$$

which evaluates to $B_r \Omega(r - r_{\min}) (\partial V'_{sw} / \partial \phi) / V'^2_{sw}$ in the heliographic equatorial plane ($\theta = 90^\circ$).

For completeness, and for later reference, this modified magnetic field's vector expression is given here as

$$\vec{B} = B_r \left(\hat{e}_r + \frac{\Omega(r - r_{\min}) \sin \theta}{V'_{sw}} \hat{e}_\phi + \frac{\Omega(r - r_{\min})}{V'^2_{sw}} \frac{\partial V'_{sw}}{\partial \phi} \frac{1 - \cos \theta}{\sin \theta} \hat{e}_\theta \right), \quad (5.15)$$

with magnitude

$$B = B_r \sqrt{1 + \left(\frac{\Omega(r - r_{\min}) \sin \theta}{V'_{sw}} \right)^2 + \left(\frac{\Omega(r - r_{\min})}{V'^2_{sw}} \frac{\partial V'_{sw}}{\partial \phi} \frac{1 - \cos \theta}{\sin \theta} \right)^2}, \quad (5.16)$$

where $B_r = B_0(r_0/r)^2$ with 5 nT employed as a typical value for B_0 at $r_0 = 1$ AU.

The modification of Eq. 5.14 is simply a measure of the compensation required for magnetic fields to remain divergence-free where $\partial V'_{sw} / \partial \phi \neq 0$. For the simple CME geometry introduced in Section 5.3, this modification therefore only has finite values within infinitesimally small intervals along the edges of the shocked flow region. The values of $\partial s / \partial \phi = s_* - 1$ translate to

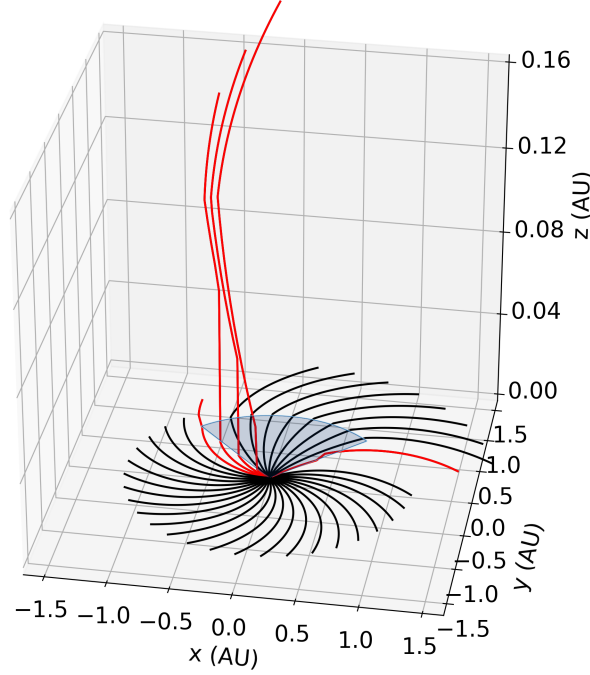


Figure 5.3: Simulated magnetic field lines constructed using $d\vec{\ell} \times \vec{B} = 0$, with $\vec{B}$ the modified field given by Eq. 5.15 for the flow speed configuration following from Eq. 5.7. The red and black lines represent field lines with and without θ -components, respectively. The shaded area represents the shocked flow speed region. Note that the scale of the z -axis is exaggerated.

B_θ -values that are at most fractions of the B_r and B_ϕ -components. As such, field lines do not make meaningful excursions out of the equatorial plane. This is illustrated in Figure 5.3 (with the z -coordinate greatly exaggerated), where field lines extend no more than 0.2 AU above the equatorial plane, out to $r = 1.6$ AU. In this case, the *Parker* [1958] field is a reasonable approximation, and the 2D transport description given in Section 5.2 remains appropriate. However, since the modification above is generally derived for any configuration where the flow speed has a longitudinal dependence, it is revisited in Chapter 6 when considering the magnetic fields associated with CIRs.

5.5 Helio-equatorial transport of CME-accelerated particles

This section illustrates how the transport of accelerated particles is altered when considered in two spatial dimensions, as opposed to the spherically symmetrical description of the previous chapter. To this end, particle intensities are simulated in two ways. Firstly, the earlier distributions of particles contributing to 1 MeV intensities during the passage of the CME shock is considered using the technique of Section 4.6.3. Secondly, the intensity profiles and energy spectra, as viewed by various observers at different positions relative to the shock's path, are also presented. All solutions are for the previously used parameters listed in Table 4.1.

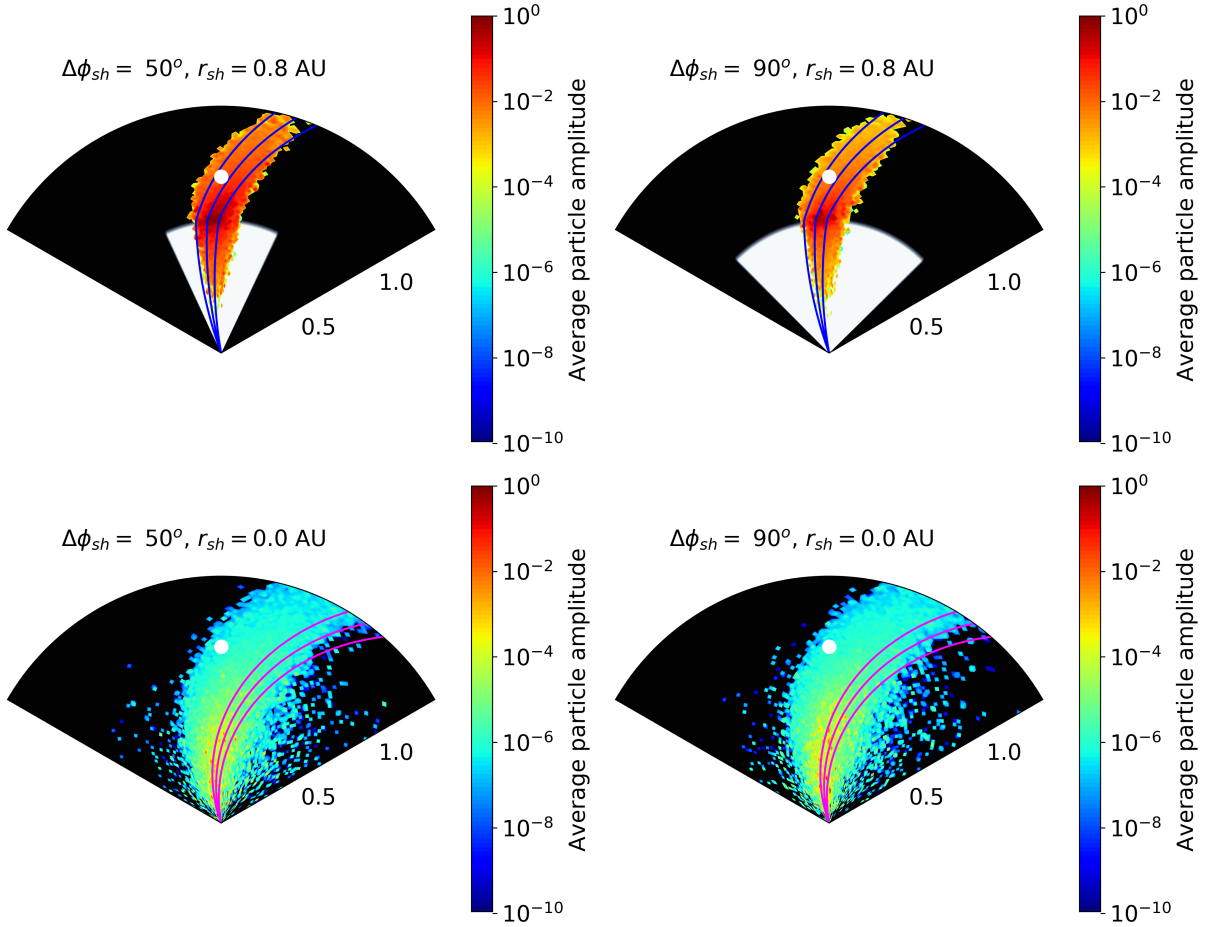


Figure 5.4: Prior distributions of particles contributing to 1 MeV intensities during the shock passage at Earth ($r = 1$ AU, $\phi = 90^\circ$; indicated by a white marker) for shocks extending $\Delta\phi_{sh} = 50^\circ$ and 90° in longitude as shown in the left and right panels, respectively. The color scale indicates normalized particle amplitudes at each point in the heliographic equatorial plane, shown for the indicated positions of the shock. The flow speeds are shown in monochromatic scale in the background, while blue or magenta lines represent sample magnetic field lines.

5.5.1 The effects of varying the longitudinal shock extent

Chapter 4 considers the acceleration of ESPs by shocks that are assumed to extend a full 360° in longitude. In such a scenario, any observer with respect to which the transport of these accelerated particles is considered would inadvertently be situated in the shock's path. The effects of shock broadness on particle intensities as viewed by an observer in the shock path, as well as the locations from where the accelerated particles are transported, is explored here.

Figure 5.4 shows the particle amplitude-weighted distributions of pseudo particles traced time-backwards from the observational point at $r = 1$ AU, $\phi = 90^\circ$ and $E = 1$ MeV. These plots map the earlier distributions of particles contributing to 1 MeV intensities at the time of the shock passage, whereas the significance of those contributions are indicated by the color scale. The distributions for $\Delta\phi_{sh} = 50^\circ$ and 90° are shown, each for two instances in time, namely, when the shock is 0.2 AU away from the observer and at its departure from near to the Sun, in the top and bottom panels of Figure 5.4, respectively. Qualitatively, the distributions for the two cases of $\Delta\phi_{sh}$ are similar. Both show that the most significant contributions emanate from near the shock front, and that particles are distributed tightly along magnetic field lines. Note also

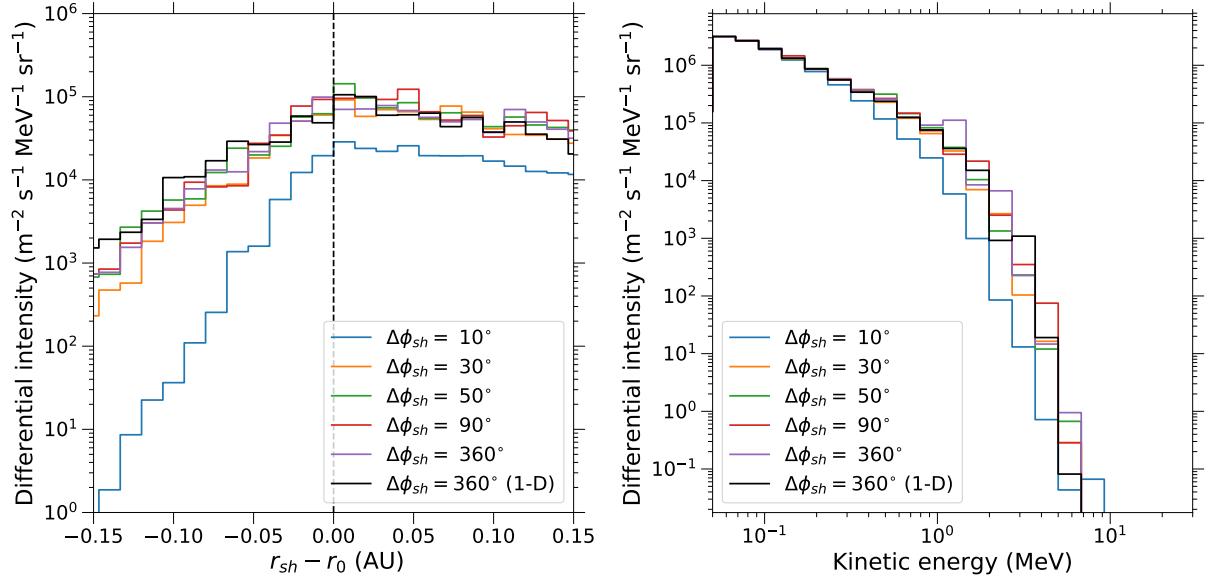


Figure 5.5: Left: Simulated profiles of 1 MeV particles during the passage of shocks of various longitudinal extents. The vertical line indicates the moment of the shock’s arrival at the observer’s position. Right: Simulated energy spectra at the moment of the shock’s arrival at the observer’s position for various longitudinal shock extents.

how the distributions and the field lines bend in a similar fashion across the shock. Therefore, considering transport strictly in the diffusive limit, these plots suggest parallel diffusion is the prevalent mechanism by which accelerated particles are transported from the shock to the observer. Whereas the initial distributions (when $r_{sh} = 0$) associated with either case of $\Delta\phi_{sh}$ are nearly identical, when $r_{sh} = 0.8$ AU the distribution for the broader shock is only marginally more concentrated at the shock front.

Similarly, in Figure 5.5, the energy spectra and time profiles of intensities as viewed by the observer at $r = 1$ AU and $\phi = 90^\circ$ respond negligibly to varying the longitudinal extent of the shock. The time profiles show the typical features of an ESP event, similar to Figure 4.17, and the energy distributions show the power laws and exponential cutoffs associated with shock-accelerated spectra. In fact, the spherically symmetrical (1D) model implemented in Chapter 4 reproduces the 2D simulations for all but the narrowest of shocks. For $\Delta\phi_{sh} = 10^\circ$, intensities are lower than for the other cases, especially at higher energies. For such a longitudinally narrow (and likely unrealistic) shock, the source region is smaller. The observer is also nearer to the longitudinal boundaries of the shock, and there may be appreciable perpendicular diffusion of accelerated particles away from field lines connecting the shock to the observer. The role of perpendicular diffusion is explored further in Section 5.5.3.

5.5.2 Accelerated particle transport near shock flanks

It is noted that while the intensities viewed by an observer in the shock’s direct path will be comprised predominantly of locally accelerated particle intensities, Figure 5.4 illustrates that particles transported to such an *in situ* observer ahead of the shock also make significant contributions. However, an observer outside the shock path would register only the intensities of remotely accelerated particles. The transport of these particles from the shock to the observer

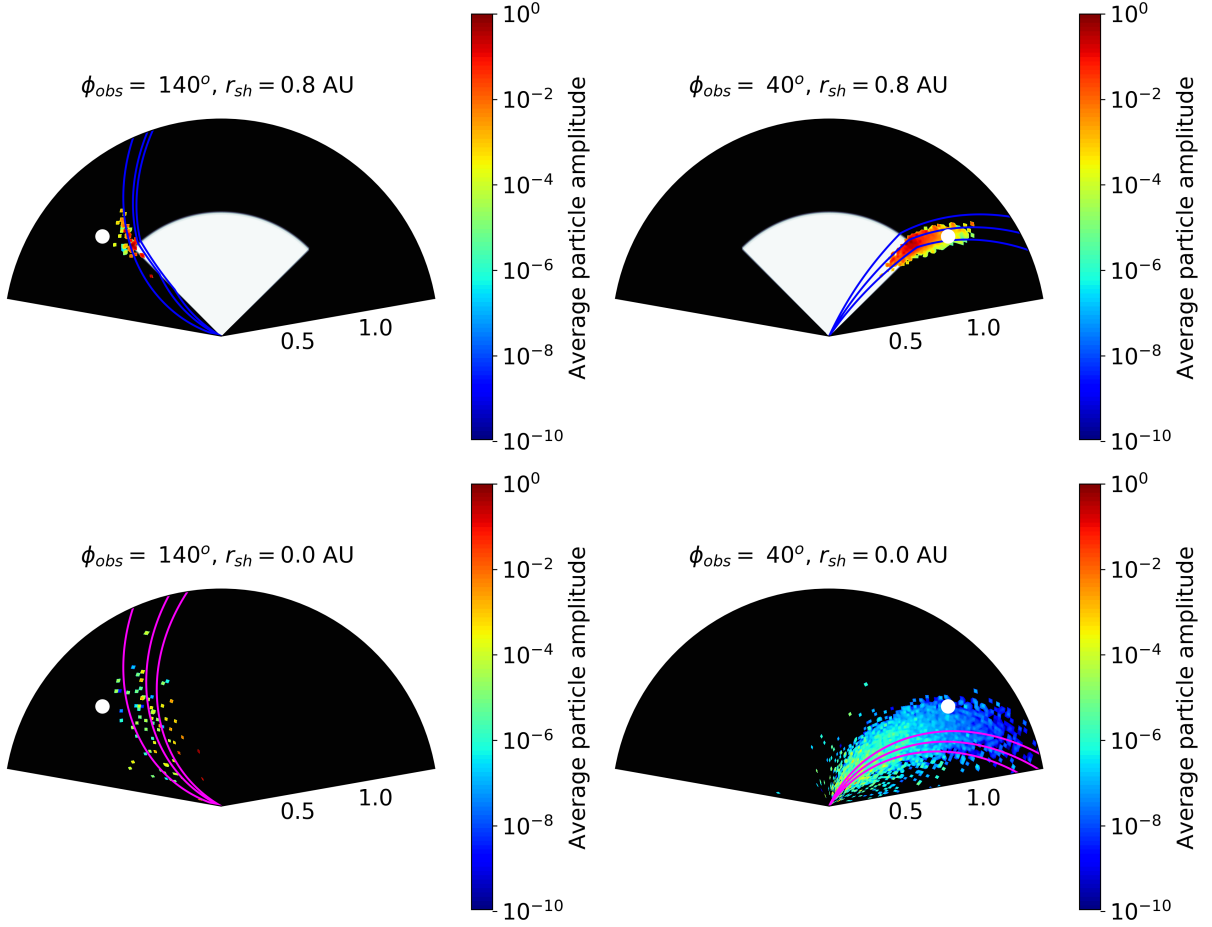


Figure 5.6: Similar to Figure 5.4 for a shock with a longitudinal extent of $\Delta\phi_{sh} = 90^\circ$, but for observers on the western and eastern flanks, at $\phi_{obs} = 140^\circ$ and 40° , as shown in the left and right panels respectively.

is furthermore dependent on the presence of favourable magnetic connections.

To investigate this concept of remote acceleration, virtual spacecraft are positioned at 1 AU outside the path of the advancing shock front (with $\Delta\phi_{sh} = 90^\circ$) on its west and east flanks, at $\phi_{obs} = 140^\circ$ and 40° , respectively. Using the same technique applied in Figure 5.4, the prior distributions of particles contributing to 1 MeV intensities at each of the aforementioned observers at the moment when $r_{sh} = r_0$ are traced backwards in time. These distributions are shown in Figure 5.6. These earlier distributions of contributing particles are vastly different for the two observers considered, owing largely to differences in the connecting field line geometry. On the east flank, for $\phi_{obs} = 40^\circ$, a direct magnetic connection exists between the shock front and the observer, and contributing particles are distributed along these connecting field lines. This is similar to the cases considered in Figure 5.4, but with the distinction that the observer at $\phi_{obs} = 40^\circ$ is never in direct contact with the shock. This also implies that intensities viewed by an observer east of the advancing shock may peak when the most optimal magnetic connection is established between the shock front and the observer, and not necessarily for the minimum distance between them. *Cane et al.* [1988] and *Reames* [1999] report similar findings.

By contrast, field lines deviate away from the observer on the west flank, implying poor magnetic connections for the whole duration of the shock's approach to 1 AU. Figure 5.6 shows that

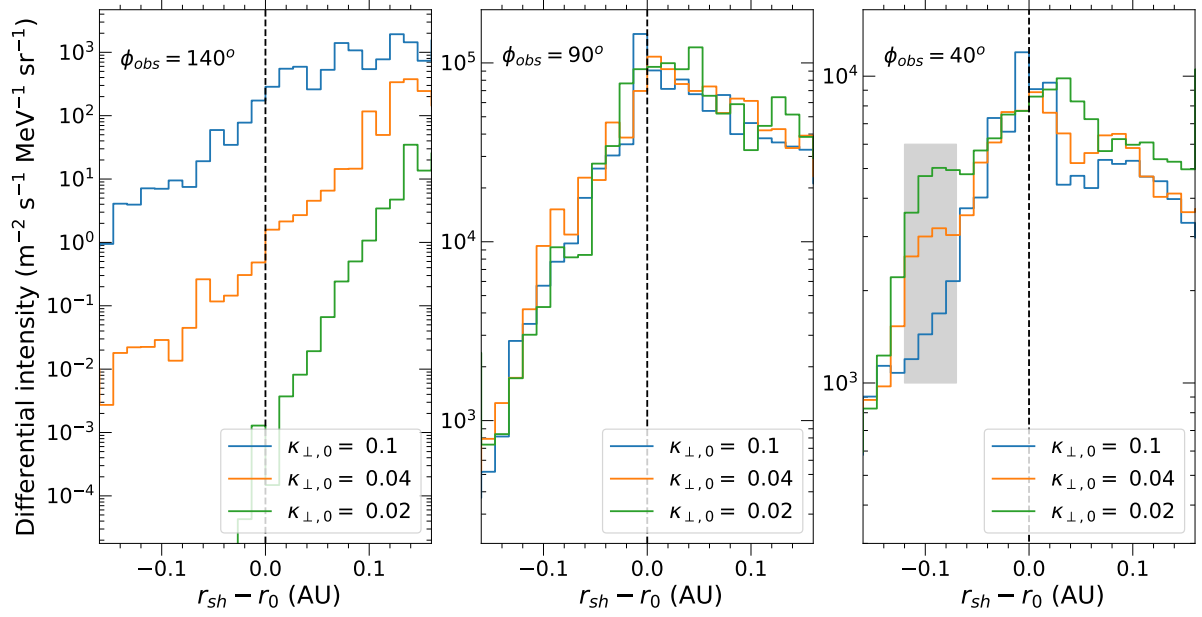


Figure 5.7: Simulated profiles of 1 MeV particle intensities as viewed by observers at different longitudes and for different levels of perpendicular diffusion. The observers corresponding to the panels from left to right are positioned at $\phi_{\text{obs}} = 140^\circ$, 90° , and 40° , and at a heliocentric distance of $r_0 = 1$ AU. The coefficient $\kappa_{\perp,0}$ is as defined for Eq. 5.6. The vertical lines indicate the shock’s arrival at 1 AU, and the shaded area indicates $\kappa_{\perp}$ -dependent intensity enhancements.

the distributions traced time-backwards from the observer at $\phi_{\text{obs}} = 140^\circ$ are also distributed along field lines, but sparsely. In this case, owing to the absence of viable magnetic connections, pseudo-particle trajectories connecting the shock front and the observer are improbable. Here, the successful transport of accelerated particles to the observer is reliant on perpendicular diffusion, which is inefficient compared to parallel diffusion as it operates on smaller length scales. However, as the shock advances beyond 1 AU, the magnetic connection could improve as the observer may be connected to the shock from behind. Indeed, the leftmost panel of Figure 5.7 shows intensities still increasing after the shock had passed 1 AU, presumably peaking at some later time.

The time profiles in Figure 5.7 for each of the observers are reminiscent of similar longitudinal variations in SEP events [e.g. Reames, 1999]. Of course, for an observer centered with regards to the shock front, and in its direct path, the time profiles are similar to those of ESP events (e.g. Figure 4.17), and intensities peak when the shock itself passes the observer. Similarly, owing to field line geometry, intensities during gradual SEP events tend to peak after the shock passage at an observer on the western flank, whereas intensities viewed by an observer on the eastern flank tend to be enhanced before the shock passage [see also Hu et al., 2017, 2018]. Qualitatively, these features are similar to those of the profiles in Figure 5.7. However, some important distinctions must be made. The first of which concerns the seed particles and their source regions. An observer on the eastern flank of a CME shock may be magnetically connected to a western solar-source longitude [e.g. Reames, 1999], but in the simplified description employed here (as discussed in Section 5.3), the large tangential magnetic field components expected behind the shock are absent, and field lines at observers connect to similar longitudes near the Sun. In this study, since particles are injected from the SW distribution anywhere along the shock front, the Sun-observer connection is less important than the shock-observer connection.

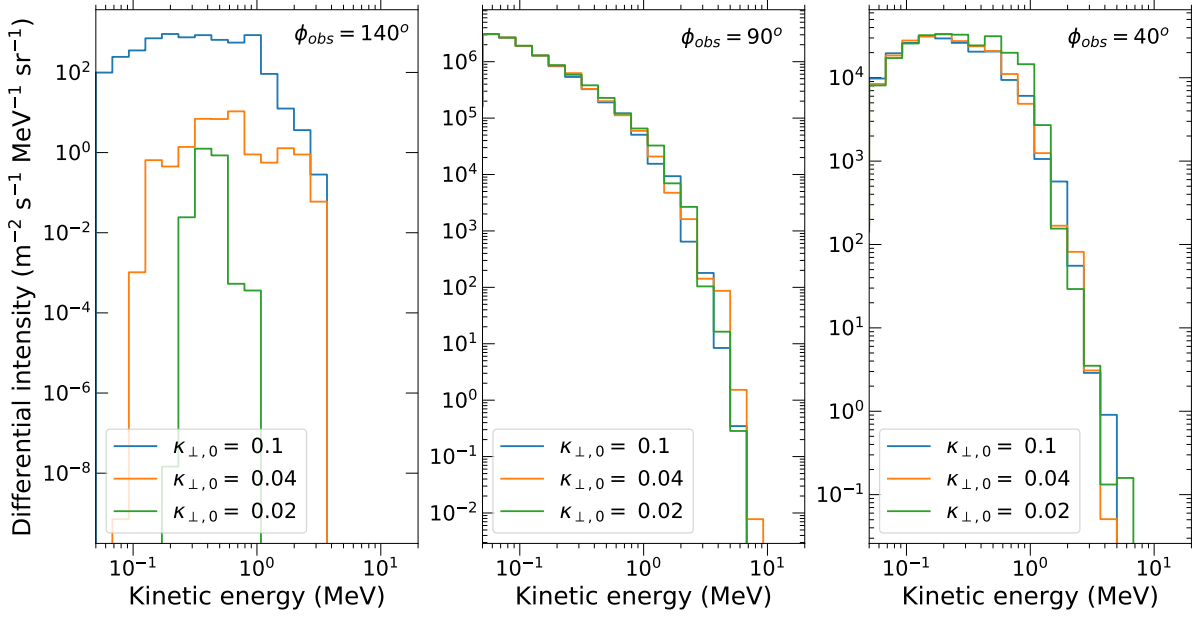


Figure 5.8: Simulated energy spectra for different values of $\kappa_{\perp,0}$ (as defined for Eq. 5.6) as viewed by the observers in the corresponding panels of Figure 5.7 at the moment of the shock’s arrival at 1 AU.

Moreover, SEP transport is often considered in the streaming limit [e.g. Hu et al., 2017, 2018], as opposed to the predominantly diffusive transport considered in this study. The latter process is notably slower, with consequences for intensity profiles. In the streaming limit, particles are transported from remote acceleration sites much faster, resulting in intensities peaking either longer before or after the shock passage for observers on the eastern and western flanks, respectively. In the diffusive limit, the shock is largely able to keep up with particles diffusing randomly along connected field lines and accelerates them continuously (as evinced by the large particle amplitudes associated with shock fronts in Figures 5.4 and 5.6). The passage of the shock itself is therefore still likely to be associated with intensity enhancements. Also, particles become less likely to reach the observer on the timescales of the shock’s propagation should the shock be further removed from the observer. The contributions of particles transported to the observer by means of diffusion is therefore more likely to result in broad intensity plateaus within a short time of the shock’s arrival rather than definitive peaks occurring either long before or afterwards.

Considered at the moment of the shock’s arrival at 1 AU, the energy spectra of Figure 5.8 viewed by observers in and out of the shock’s path reveal quintessential features of locally and remotely accelerated particles, respectively. In the central panel of Figure 5.8, the power-law distribution rolling over into an exponential decrease at high energies are the typical spectral features of particles accelerated *in situ* by means of DSA as the shock sweeps over the observer (similar to the spectra presented in Chapter 4). The observers that are not in the shock’s direct path observe modulated versions of the aforementioned spectrum. Here, all of the contributing particles are transported from remote acceleration sites along the shock front. For instance, the spectra viewed by the observer on the eastern flank of the shock, at $\phi_{\text{obs}} = 40^\circ$, resemble those of Figure 4.16, where similar low-energy downturns are observed as a result of the disproportionate modulation of low-energy particles owing to e.g. rigidity-dependent diffusion. The modulation of remotely accelerated particle spectra is more severe in the diffusive limit, owing

to higher scattering rates and longer times spent by particles in transit. By contrast, the results of focused transport models show that the time-integrated fluences of SEP protons transported from remote shock-acceleration sites tend to retain power-law forms [Hu *et al.*, 2017, 2018].

5.5.3 Relative importance of parallel and perpendicular diffusion

From the above discussions, diffusion along magnetic field lines is evidently an important transport process, whereas perpendicular (or cross-field) diffusion is shown in *e.g.* the left panel of Figure 5.6 to be inefficient by comparison. However, for the observer on the western flank of the shock, at $\phi_{\text{obs}} = 140^\circ$, the transport of accelerated particles is reliant on perpendicular diffusion, since there are no field lines adequately connecting the shock and the observer. This section therefore illustrates the relative importance of perpendicular diffusion for observers at different positions relative to the shock as introduced in Figures 5.4 and 5.6.

The relative magnitudes of the perpendicular diffusion coefficients are varied for the simulations shown in Figures 5.7 and 5.8. It is evident that for the observers either directly in the shock path ($\phi_{\text{obs}} = 90^\circ$) or magnetically connected to the shock ($\phi_{\text{obs}} = 40^\circ$), intensities do not generally vary in response to varying $\kappa_{\perp,0}$, with the different solutions corresponding within the margins of stochastic variations. One apparent exception is visible for the observer on the eastern shock flank during the approach of the shock. The shaded area in the rightmost panel of Figure 5.7 shows appreciable enhancements of intensities for smaller $\kappa_{\perp,0}$ -values. Less perpendicular diffusion better confines particles near the shock, which facilitates more efficient acceleration. Because the transport of accelerated particles to the observer at $\phi_{\text{obs}} = 40^\circ$ is furthermore entirely reliant on the shock-observer magnetic connection, larger perpendicular diffusion facilitating transport away from this magnetic connection results in lower intensities at the observer's position.

By contrast, the transport of accelerated particles to the observer on the western flank of the shock, at $\phi_{\text{obs}} = 140^\circ$, is shown in Figures 5.7 and 5.8 to be heavily reliant on increased perpendicular diffusion. In fact, the leftmost panel of Figure 5.8 shows intensities are much lower if perpendicular diffusion coefficients are small. In this case, particles must be transported by means of cross-field diffusion from the shock front, or field lines connected to the shock front, because the observer is neither magnetically connected nor in the path of the shock itself. Note that while perpendicular diffusion is the most important mechanism for transporting particles to this observer, the relative inefficiency of this process is demonstrated by the low intensities compared to those observed at the opposite flank of the shock.

5.6 Summary and conclusions

This chapter introduces a simple longitudinally dependent CME shock to illustrate features of the transport of accelerated particles in the heliographic equatorial plane. Despite the inclusion of a correction to ensure the SW-embedded magnetic field is divergence-free in longitudinally varying flow speed regions, the magnetic field remains appreciably *Parker* [1958]-like, allowing

the TPE to be solved for only two spatial coordinates, namely r and ϕ . This simple model configuration reveals a number of insights that are pertinent to the multi-dimensional spatial transport of accelerated particles generally.

Firstly, it is shown that an observer situated directly within the path of a travelling shock observes the typical intensity profiles associated with ESP events, with spectra produced at the moment of the shock's arrival resembling those predicted by DSA. For such observers, it is shown that the transport of particles associated with shocks of varying longitudinal extents may be adequately described using a spherically symmetrical model. An exception to this arises when shocks are narrow enough for particles to be transported away from regions that are magnetically connected to the source region by means of cross-field diffusion. Secondly, the features of particles that are transported to the observer from remote acceleration sites, along shocks of finite longitudinal extents, are also considered. For these observers, spectra resemble modulated forms of those associated with ESP events, most often with low-energy downturns owing to low energy particles being more susceptible to modulation during their transport from remote acceleration sites. The evolution of intensity profiles for these observers depends on the arrangement of the magnetic field.

For observers outside the direct path of the shock, but magnetically connected to the advancing shock front, particles are predominantly transported to the observer by means of parallel diffusion. Such magnetic connections readily occur on the eastern sides of propagating CMEs, owing to the corotation-induced curvature of magnetic field lines. It is noted that the intensities at these observers may be enhanced ahead the shock's closest approach should favourable magnetic connections be established at an earlier time. Moreover, enhanced perpendicular diffusion is shown to dampen these early intensity enhancements, because particles are transported away from the field lines connecting the observer with the shock. By contrast, perpendicular diffusion is essential to transport particles from the shock to those observers (typically on the western side of CMEs) that are not magnetically connected to the shock. However, owing to perpendicular diffusion being comparatively inefficient, intensities are notably lower for these observers than for those that are magnetically connected. The presence of magnetic connections therefore serves as a major organizing factor in the longitudinal distributions of accelerated particle intensities.

While the simulated intensity profiles viewed by the various observers considered here bear some resemblance to those observed during gradual SEP events, differences exist with regards to how particles are transported. As opposed to SEP transport, which is most often considered in the streaming limit, the current study considers transport in the diffusive limit. Parallel diffusion is a comparatively slow process, and therefore intensity enhancements associated with particles transported to the observer along field lines would occur within a short time of the shock's closest approach, as opposed to peaking either long before or afterwards for streaming SEPs. Nevertheless, it is established that the transport of at least some component of remotely accelerated particles can be simulated successfully in the diffusive limit as well.

The concepts of remotely accelerated particles and the prominent role of the magnetic field in their transport are also pertinent to the study of acceleration associated with CIR shocks. This is explored in Chapter 6. It is noted finally that particle drifts may also affect transport in the ϕ -

direction, which, in turn, may affect transport relative to magnetic connections. However, drifts are largely reduced by turbulent fluctuations for the low-energy particles considered here, and are therefore not expected to have an appreciable effect.

Chapter 6

Particle acceleration in corotating interaction regions

6.1 Introduction

Energetic particles can be accelerated up to MeV energies at shocks associated with CIRs [Barnes and Simpson, 1976; Fisk and Lee, 1980], likely by means of DSA [Lee and Fisk, 1982; Scholer et al., 1999]. The intensities of CIR-accelerated particles typically peak in the compressed fast stream of interaction regions near the trailing edge, and scale according to local compression ratios [Desai et al., 1998; Ebert et al., 2012]. These results suggest that particles are accelerated locally at the trailing edge. However, at 1 AU, these features were also observed in the absence of shocks at the trailing edge [Richardson and Zwickl, 1984; Desai et al., 1998; Chottoo et al., 2000; Ebert et al., 2012], suggesting magnetically-connected sources beyond Earth's orbit [Fisk and Lee, 1980; Scholer et al., 1999]. Indeed, evidence exists for the sunward streaming of CIR particles [e.g. Richardson et al., 1993], linking their high abundances observed in the high-speed stream near Earth to acceleration by reverse shocks at CIR trailing edges located at a few AU [see also Richardson, 2018].

As a result of the modulation of particles being transported to Earth against the expanding SW, which disproportionately affects low-energy particles, a low-energy turnover in spectra is expected [e.g. Fisk and Lee, 1980]. However, this is not generally observed, and spectra extend down to energies of ~ 10 –100 keV, often behaving like a power law [Mason et al., 1997, 1999]. Since these spectra appear to merge with the SW distribution [e.g. Chottoo et al., 2000], CIR particles observed at 1 AU in the absence of a shock may be accelerated more locally from the suprathermal SW as opposed to being transported from remote shocks [Filwett et al., 2017; Yu et al., 2017]. Observations of particles abundances in CIR events support a source based in the suprathermal SW [Mason et al., 2008, 2012; Bučík et al., 2012; Filwett et al., 2017].

In this chapter, the suprathermal tail of the SW is assumed to be a general seed population for energetic CIR particles. Their acceleration is considered during CIR passages, and strictly within the diffusive limit, involving either DSA at shocks associated with CIR edges or acceleration by converging scattering centres inside the CIR [Jokipii et al., 2001; Giacalone et al., 2002]. The aim is to investigate the extent to which these acceleration mechanisms can account for

observed features of CIR particles, and particularly the organization of their peak intensities and spectral indices (See Sections 6.4 and 6.6). To this end, an analytical description of the CIR properties is introduced in Section 6.2, which includes a discussion of the related SW energy distribution, while Section 6.3 details the modelling of CIR particle acceleration. Finally, the contributions of non-locally accelerated particles are discussed in Section 6.7.

Note that even though compression waves at large heliocentric distances, where their propagation speeds may exceed magnetosonic speeds, may qualify as shocks, they may nevertheless be referred to as *compression waves* to keep discussions concerning them general.

6.2 Modelling the solar wind in CIRs

In order to study particle acceleration within compressed SW regions, Jokipii *et al.* [2001] introduced an analytical description for the SW flow speed to describe CIR-associated compressions, which resemble either the forward or reverse compression of a CIR depending on the relative configurations of the flow and compression speeds [see also Giacalone *et al.*, 2002]. In the present study, this description is expanded to describe an interaction region bounded by compression waves at both edges, with the aim of investigating the relative contributions of particle acceleration at each of them. This is achieved by expressing the radial SW flow speed, in a frame corotating with the Sun at an angular speed of $\Omega_\odot = 2.67 \times 10^{-6} \text{ rad s}^{-1}$, as follows:

$$V'_{sw} = V'_S + \frac{1}{2} (V'_{SF} - V'_S) \left(\tanh \left(\frac{\phi + r\Omega_\odot/W_{LE} - \phi_{rf}^{LE}}{\Delta\phi_{rf}^{LE}} \right) - \tanh \left(\frac{\phi + r\Omega_\odot/W_{LE} - \phi_c^{LE}}{\Delta\phi_c^{LE}} \right) \right) + \frac{1}{2} (V'_F - V'_S) \left(\tanh \left(\frac{\phi + r\Omega_\odot/W_{TE} - \phi_{rf}^{TE}}{\Delta\phi_{rf}^{TE}} \right) - \tanh \left(\frac{\phi + r\Omega_\odot/W_{TE} - \phi_c^{TE}}{\Delta\phi_c^{TE}} \right) \right). \quad (6.1)$$

Here, V'_S and V'_F represent the fixed-frame flow speeds of the uncompressed slow and fast SW, respectively, while V'_{SF} is used to define an intermediate flow speed transition inside the interaction region. The quantities $\Delta\phi_c$ and ϕ_c represent the azimuthal width and position of compression waves associated with either the leading edge (*LE*) or trailing edge (*TE*) of the CIR, while $\Delta\phi_{rf}$ and ϕ_{rf} define the same for the associated rarefaction regions. The constants W_{LE} and W_{TE} can be interpreted, respectively, as the speeds at which the leading and trailing edge compression waves propagate radially outward in the inertial frame. Note that since the CIR is drawn out by corotation, it can extend for several revolutions. Eq. 6.1 is therefore defined for $\phi \in (-\infty, \infty)$. The value of ϕ should *not* be adjusted to the $[0^\circ, 360^\circ)$ domain for $\phi \geq 360^\circ$.

For the present study, the following assumptions are made with regards to the aforementioned parameters: the azimuthal positions of the compression and rarefaction regions for the two edges are related according to

$$\phi_{rf}^{TE} = \phi_{rf}^{LE} + 10^\circ \quad \text{and} \quad \phi_c^{TE} = \phi_c^{LE} + 10^\circ, \quad (6.2)$$

which ensures the correct structure of the CIR at $r \lesssim 1 \text{ AU}$ (see Section 6.2.1). Furthermore, the azimuthal separation between compression and rarefaction regions is kept fixed at $\phi_c - \phi_{rf} =$

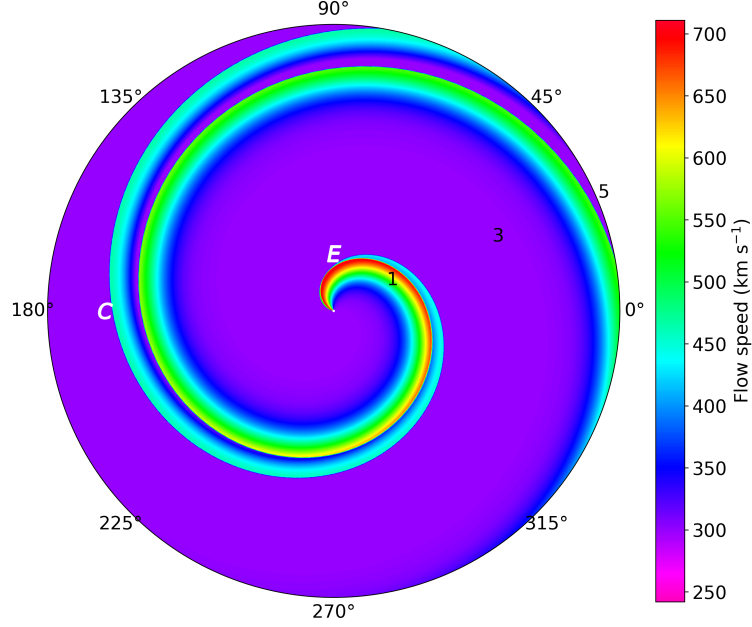


Figure 6.1: Colour-scaled plot of the SW flow speed in the heliographic equatorial plane out to 5 AU as described by Eq. 6.1 for the reference parameters $\phi_c^{LE} = 160^\circ$, $\Delta\phi_c^{LE} = \Delta\phi_c^{TE} = 0.5^\circ$, $V_F' = 600 \text{ km s}^{-1}$, and $V_{SF}' = 480 \text{ km s}^{-1}$. The markers E and C represent observers at the coordinates $(r, \phi) = (1 \text{ AU}, 90^\circ)$ and $(4 \text{ AU}, -180^\circ)$, for which the time profiles of various SW quantities are considered throughout Section 6.2.

30° for both edges. With the aforementioned coupling of parameters, a time dependence can be simulated in Eq. 6.1 by varying only ϕ_c^{LE} with time at the corotation rate of $\Omega_\odot$. While the widths $\Delta\phi_{rf}^{TE} = 40^\circ$ and $\Delta\phi_{rf}^{LE} = 20^\circ$ and speeds $W_{LE} = 260 \text{ km s}^{-1}$, $W_{TE} = 220 \text{ km s}^{-1}$, and $V_S' = 300 \text{ km s}^{-1}$ are assumed to be fixed, the parameters $\Delta\phi_{rf}^{LE}$, $\Delta\phi_{rf}^{TE}$, V_F' , and V_{SF}' are varied depending on the application considered.

With the aim of simulating SW energy distributions by using κ -functions, it is also necessary to characterise the densities and temperatures within CIRs. To this end, the equations introduced in Section 4.3.1 are applied again, with the SW number density (Eq. 4.14) as derived from the continuity equation, and the temperature according to the expressions in Eqs 4.15 to 4.17. Recall that in those expressions the flow speeds are transformed to the shock frame. For the single compression-wave model of *Giacalone et al.* [2002], the shock speed can be readily calculated using the ratio of the radial and azimuthal flow speed gradients and is the equivalent of either W_{LE} or W_{TE} . However, the compression waves associated with the CIR in Eq. 6.1 are specified to move at two different speeds. For simplicity, an average radial speed, representative of the whole CIR structure, and defined as

$$W_{ave} = \frac{1}{2} (W_{TE} + W_{LE}) \quad (6.3)$$

is substituted for V_{sh} in the expressions for the SW number density and temperature. Parameters in the current configuration, where $W_{TE} < W_{LE} < V_S'$, should generally be chosen such that $V_{sw}' > W_{ave}$ to avoid singularities and negative values. The uncompressed slow SW speed and a density far ahead of the CIR are chosen as reference values, such that $V_0 = V_S'$ and $n_0 = 0.24 \text{ cm}^{-3}$ at $r_0 = 5 \text{ AU}$ (which corresponds to $\sim 6 \text{ cm}^{-3}$ at 1 AU). The following subsections illustrate the features of CIRs simulated using the above analytical description.

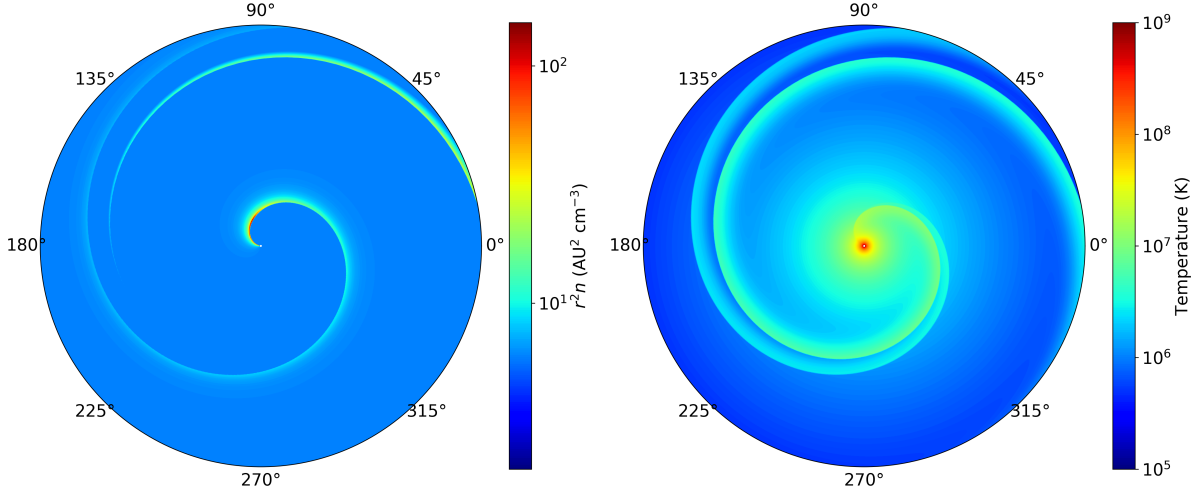


Figure 6.2: Scaled number densities ($r^2 n$) and temperatures (T) corresponding to the simulated flow speeds shown in Figure 6.1.

6.2.1 Comparison with features from observations and simulations

The structure of the CIR according to Eq. 6.1 is illustrated in Figure 6.1 in the heliographic equatorial plane. This is for parameters $\phi_c^{LE} = 160^\circ$, $\Delta\phi_c^{LE} = \Delta\phi_c^{TE} = 0.5^\circ$, $V_F' = 600 \text{ km s}^{-1}$, and $V_{SF}' = 480 \text{ km s}^{-1}$. *Note these are reference parameters used in all following applications, unless specified otherwise.* This analytically modelled CIR displays the most noticeable large-scale flow speed features of those rendered using MHD simulations [e.g. *Wiengarten et al., 2014; Wijzen et al., 2019*].

Figure 6.1 shows the CIR as a spiral-like structure in the corotating frame. At smaller radial distances, nearer to the solar disk, a high-speed stream with flow speeds $\gtrsim 600 \text{ km s}^{-1}$ is observed, which diminishes further along the spiral as two distinct flow structures emerge. Each of these flow structures is bounded by a compression wave at its outer boundary, and a broader rarefaction region associated with more gradually decreasing flow speeds, behind it. For the outer flow structure at the leading edge of the CIR the compression wave represents a forward compression, whereas the compression wave associated with the inner flow structure, at the trailing edge of the CIR, represents a reverse compression. As time progresses, the CIR propagates radially outward and rotates in a counter-clockwise direction as viewed from the solar north pole. However, since the aforementioned flow structures at the leading and trailing edges are specified to move at different radial speeds in the inertial frame, namely W_{LE} and W_{TE} , the separation between them increases with radial distance, thereby widening the CIR.

The geometrically scaled number densities and temperatures corresponding to the flow speeds in Figure 6.1 are shown in Figure 6.2. The number densities in this plot are scaled to suppress their strong radial dependence and accentuate changes owing to flow speed variations in the CIR. For the considered configuration, number densities are large in two distinct compressed SW regions associated with slower flow speeds. At smaller heliocentric distances, densities are noticeably enhanced ahead of the leading edge, whereas a similar enhancement ahead of the trailing edge becomes more pronounced further along the CIR. Aside from its pre-existing radial dependence, the temperature scales in a manner similar to the flow speed in the CIR and

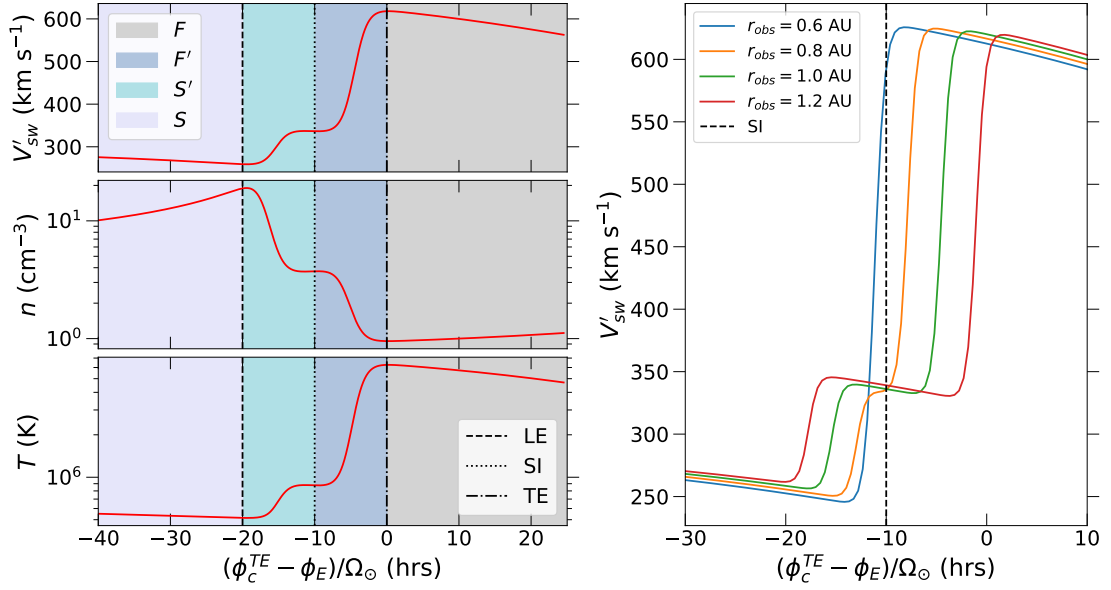


Figure 6.3: Left: Time profiles simulating the change in SW flow speed (V'_{sw}), number densities (n) and temperatures (T) during the passage of the CIR. These are shown for the same parameter configuration in Figure 6.1, but with $\Delta\phi_c^{LE} = \Delta\phi_c^{TE} = 1^\circ$ and $V'_{SF} = 390$ km s⁻¹. Regions shaded in different colors, as indicated in the legend in the top panel, represent different flow regions: S represents the ambient, unperturbed slow SW, S' the compressed, accelerated slow SW, F' the compressed, decelerated fast SW stream, and F the unperturbed fast SW stream. The vertical lines represent boundaries between distinct flow regions, namely the leading edge (dashed line), stream interface (dotted line), and the trailing edge (dash-dotted line). Right: Time profiles of flow speeds seen by observers at the positions shown in the legend, superimposed on the flow speed as viewed by the observer at 1 AU, simulating the formation of compression waves bounding the SI. The observer at $r_{obs} = 1.2$ AU is at $\phi = 70^\circ$, while the rest are at 90° . The time axes are defined according to the angular separation of the trailing edge ϕ_c^{TE} and the observer ϕ_E , with $\Omega_\odot$ the corotation rate.

is higher where the SW is fast [see also Gosling *et al.*, 1972].

To demonstrate the model's representation of observed characteristics, time profiles of the plasma quantities discussed above are illustrated from the perspective of an observer at Earth. The left panel of Figure 6.3 shows the simulated evolution of flow speeds, number densities and temperatures as viewed by an observer at Earth in the heliographical equatorial plane. These profiles are illustrated as a function of the time either until or since the arrival of the CIR trailing edge, and correspond to the CIR rotating through 40° across the observer, where $\phi_c^{LE} = 160^\circ \rightarrow 200^\circ$. They are shown for the same parameter configuration as in Figure 6.1, but with $\Delta\phi_c^{LE} = \Delta\phi_c^{TE} = 1^\circ$ and $V'_{SF} = 390$ km s⁻¹. Distinct regions of different flow properties are distinguishable. These correspond to those identified by Belcher and Davis [1971] in Mariner 5 spacecraft observations. The undisturbed slow SW (denoted S in Figure 6.3) transitions across the leading edge of the CIR to a region of compressed and somewhat accelerated flow (S') due to its interaction with the fast SW stream. Similarly, across the trailing edge, the fast SW stream (F) transitions to a compressed and decelerated flow region (F') as a result of the aforementioned interaction with the slow SW.

These perturbed slow and fast SW regions constitute the stream interaction region (SIR). See Richardson [2018] for a complete review of related observations. With regards to the other quantities, density enhancements inside SIRs are observed to occur early in regions of positive flow

speed gradients [Gosling *et al.*, 1972, 1981], while thermal speeds largely follow the behavior of the flow speed itself [Belcher and Davis, 1971; Burlaga and Ogilvie, 1973]. Likewise, the simulated number densities peak near the leading edge, where flow speeds are depressed, while simulated temperatures (related to the thermal speed) scale similarly to the flow speed. These simulated quantities therefore resemble their counterparts in observations. The enhanced temperatures and consequently large thermal pressures in regions with faster flow speeds facilitate their expansion into the ambient slow SW.

The SIR is separated between the slow and fast SW flow regions by the stream interface [SI; Gosling *et al.*, 1978; Schwenn, 1990; Forsyth and Marsch, 1999]. At small heliocentric distances the radial flow speed at this interface takes the form of a tangential discontinuity, which becomes wider with distance [see *e.g.* Gosling *et al.*, 1978]. At $r \gtrsim 2$ AU, the development of shocks bounding the SI becomes commonplace [Gosling *et al.*, 1976; Hundhausen and Gosling, 1976; Smith and Wolfe, 1976], although these shocks have also been observed near 1 AU, albeit infrequently [Jian *et al.*, 2006]. The model of Eq. 6.1 also captures this behavior, as shown in the right panel of Figure 6.3. The time profiles of flow speeds as detected by various observers are superimposed on the flow speed as viewed by the observer at 1 AU represented on the left. Indeed, at smaller r , the radial flow speed at the SI resembles a hyperbolic tangent, which widens with increasing r along with the formation of bounding compression waves. Also note that as a result of this effect, the large flow speeds near the SI also diminish with increasing r , which simulates to an extent the disappearance of the high-speed streams which are usually visible near the Sun [Schwenn, 1990]. The onset of this effect can also be configured in Eq. 6.1 to occur further along the CIR (and hence at larger radial distances) by increasing the offset between the azimuthal positions of the compression waves in Eq. 6.2.

Aspects concerning the SI that Eq. 6.1 cannot account for are discussed in Section 6.2.2, while the discussion of SW properties continues in Section 6.2.3 for $r \geq 2$ AU.

6.2.2 Advantages and limitations of an analytical model

In this study it is assumed that the magnetic field is frozen into the plasma flow and hence convected outward with the SW. According to this principle, magnetic field lines cannot cross into regions of different plasma regimes, *e.g.* from a fast SW stream into the ambient slow SW [Gosling and Pizzo, 1999]. The faster and slower flows are consequently deflected at the SI and lead to the development of oppositely oriented non-radial flow speed components on either side of this boundary [*e.g.* Belcher and Davis, 1971]. However, as previously discussed, the SW flow is also assumed to be spherical in the inertial frame for the purposes of this study. Eq. 6.1 only characterizes the radial flow speed, while an azimuthal flow component arises only as a result of corotation. The non-radial flow components that are supposed to arise owing to deflection at the SI are therefore not accounted for when using this analytical CIR description. Furthermore, adopting Eq. 6.1 implies that plasma parcels from the same footpoint have different flow speeds as they propagate outward from the Sun. Whereas this may enhance local acceleration, because particles moving along particular magnetic field lines experience flow speed variations, it also causes field lines to intersect the SI. The SI properties are therefore only

partially represented in this description. Note that the associated magnetic field properties of this description are discussed in Section 6.3.3.

Another limitation involves the absence of the self-consistent steepening of compression waves into shocks. The compression waves bounding the interaction region are expected to steepen into shocks at the point where their own speeds exceed the magnetosonic speed, which in the SW decreases with increasing distance from the Sun. Shocks are consequently detected more readily at CIRs at larger heliocentric distances [Gosling *et al.*, 1976; Hundhausen and Gosling, 1976; Smith and Wolfe, 1976]. While a spatial dependence for $\Delta\phi_c$ in Eq. 6.1 for either edge of the CIR may emulate this steepening process, it is superfluous to the purposes of the present study, which is focused on predominantly local acceleration during the passage of a single section of the CIR past an observer. The quantity $\Delta\phi_c$ is therefore chosen accordingly on a case-by-case basis. With regards to particle acceleration, the effect of this steepening process is simulated implicitly by the radial dependence of diffusion coefficients as discussed in Section 6.3.2.

Furthermore, whereas numerically simulated CIRs [*e.g.* Wiengarten *et al.*, 2014; Wijsen *et al.*, 2019] may be better suited for large scale realistic reproductions of plasma and magnetic field observations, an analytical description presents computational advantages in the context of the present study. Firstly, given that SDEs are implemented, an analytical function for the SW speed can be invoked specifically in regions sampled by pseudo particles. Compared to using MHD models to simulate the entire projected modulation space (of which some regions may not be sampled), and subsequently coupling the output with transport models, an analytical function used to characterize the SW only along the pseudo particle trajectories is less computationally demanding. This approach also allows for greater flexibility to vary parameters. Notwithstanding its aforementioned limitations, all the information required to model the injection and acceleration processes at CIRs is derived from Eq. 6.1, including the source particle distributions discussed in Section 6.2.3. See also Vogt *et al.* [2015] and the references therein for other analytical CIR descriptions.

6.2.3 Evolution of the SW distribution during CIR passages

Following the same approach used in Section 4.3.2 for CME-driven shocks, the SW energy distribution, characterized using the κ -function of Eq. 2.5, is specified as a source spectrum for particles accelerated at CIRs. Figure 6.4 shows the spatial dependence of 60 keV SW particle intensities as described by the κ -function. As a result of the normalization of f_{κ} , this spatial distribution resembles that of the number density and displays a strong radial dependence. Figure 6.4 also shows the spiral-arm structure visible in Figures 6.1 and 6.2 in the flow speed and temperature, respectively.

Figures 6.5 and 6.6 show the evolution of the radial SW flow speed, number density and temperature as viewed by observers at Earth and further along the CIR ($r = 4$ AU, $\phi = -180^\circ$), respectively, along with the SW energy distribution at different instances during the CIR passage. These figures are analogous to Figure 4.3, and their discussions follow similarly. For the observer at Earth, the profiles shown in Figure 6.5 are similar to those in Figure 6.3, however with $\Delta\phi_c^{LE} = \Delta\phi_c^{TE} = 0.5^\circ$ and $V_{SF}' = 480$ km s $^{-1}$ such as for Figure 6.1. The number

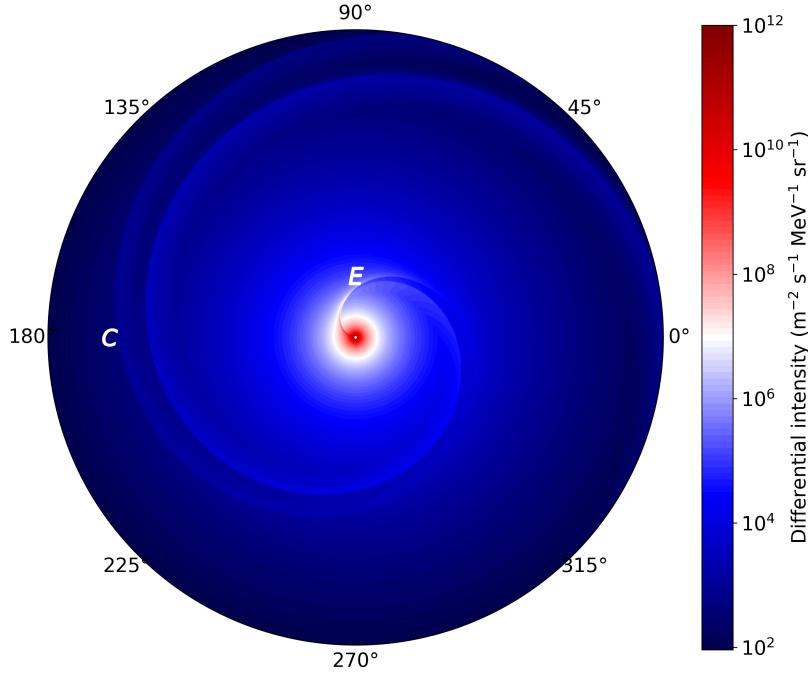


Figure 6.4: The spatial distribution of 60 keV SW particle intensities as described by Eq. 2.5 and corresponding to the flow speed, density and temperature configurations of Figures 6.1 and 6.2. The observers *E* and *C* are also as defined for Figure 6.1.

density peaks approximately 15 to 20 hours before the arrival of the trailing edge, roughly corresponding to the passage of the leading edge of the CIR. This corresponds to higher thermal peak intensities in the SW distribution. Following this, approximately 10 hours before the arrival of the trailing edge, the density has decreased by roughly an order of magnitude. The thermal peak intensity decreases as a result, while the peak itself shifts to higher energies and the overall distribution broadens in response to the accompanying increase in flow speed and temperature, respectively. Following the arrival of the trailing edge of the CIR, the flow speed and temperature have further increased, whereas the number density has decreased, albeit by a smaller amount than before. Owing to this, the SW distribution broadens and shifts further to the right. Note that following the CIR passage the intensities in the SW suprathermal tail are observed to be higher [see also *Gloeckler, 1999; Yu et al., 2018*].

For observer *C* in Figure 6.4, further along the CIR, the SW quantities evolve differently during the CIR passage. Firstly, the simulated CIR at 4 AU is appreciably wider and takes ~ 4 days to pass the observer, as opposed to roughly 1 day near Earth. As a result of the smaller magnetosonic speeds at these larger distances, compression waves bounding interaction regions typically become sharper or steepen into shocks. Likewise, large jumps in SW quantities are visible in Figure 6.6. The flow speed abruptly increases from the slow SW to the SIR at the leading edge, while decreasing from the fast stream into the SIR at the trailing edge, respectively resembling forward and reverse shocks. As a result of the interaction of the slow and fast streams, flow speeds decrease more gradually in the time between edge passages, which yields time profiles similar to those observed by *e.g. Pioneer 10* for sequential SIR edge passages at ~ 4 AU [*e.g. Hundhausen and Gosling, 1976*]. The other quantities change in relation to the flow speed as previously discussed.

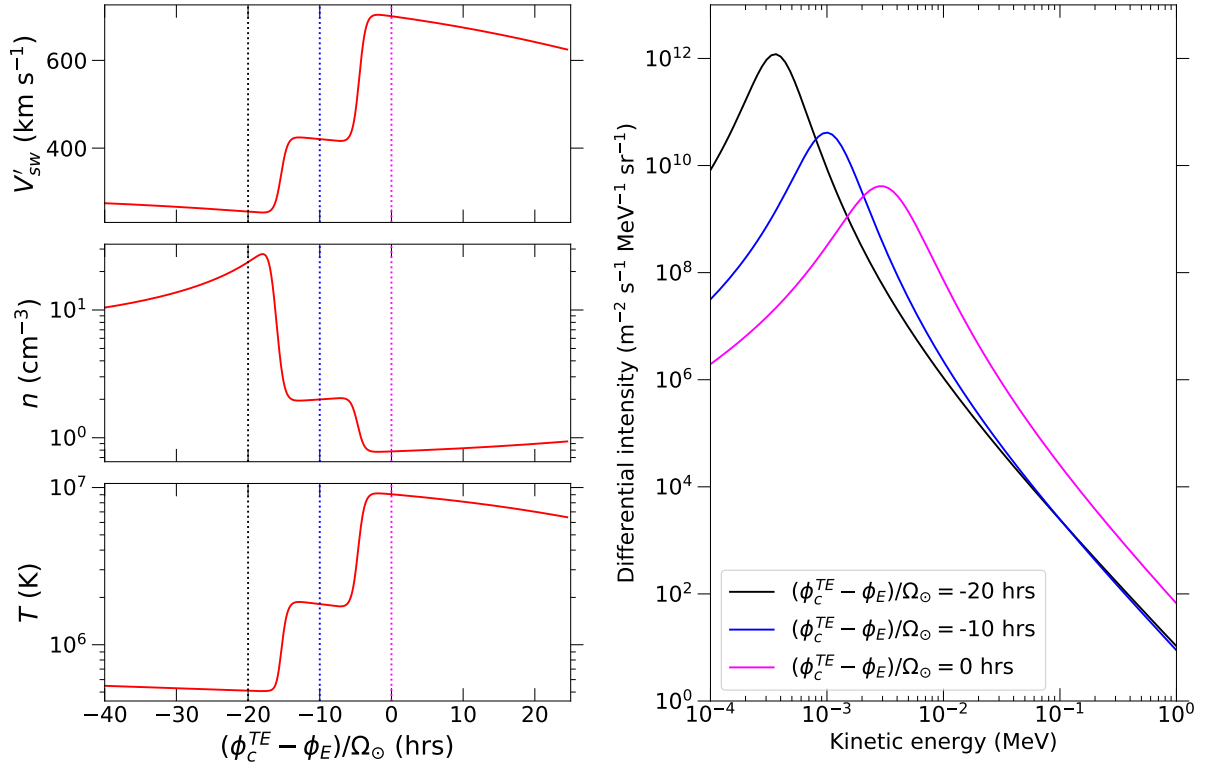


Figure 6.5: Similar to Figure 4.3, where the profiles of SW quantities as viewed by an observer at Earth are given on the left, but as a function of time relative to the CIR trailing edge arrival as defined for Figure 6.3. The associated SW energy distributions are given on the right, where curves correspond to the times indicated using vertical lines of similar colours on the left.

In Figure 6.6, preceding each of the large flow speed increases, the SW energy distribution is narrow with a large thermal peak intensity. This corresponds to lower temperatures and large number densities. Following the edge passages, the distributions have their thermal peaks shifted to higher energies in response to flow speed increases and widen following similar temperature increases. Similar to the SW distributions at Earth in Figure 6.5, suprathermal intensities are increased following the passage of either edge of the CIR. The implication of this is that more seed particles could potentially overcome injection energy thresholds for the DSA process.

6.3 Simulating CIR particle acceleration

To model the acceleration of energetic particles at SW compression regions associated with CIRs, as well as their subsequent transport, the *Parker* [1965a] TPE is applied once more with the SW flow speed as specified by Eq. 6.1. Presented simulations are mainly based on the 3D SDE solutions of Eq. 3.23, although following their comparison in Section 6.5, SDE solutions of the 2D TPE of Eq. 5.2 are presented in Section 6.6 as well. The following conditions are imposed with regards to spatial coordinates: the outer boundary of the r coordinate is set at 5 AU, while its boundary conditions are as previously defined. No boundary conditions are imposed on ϕ due to the requirement of Eq. 6.1 that $\phi \in (-\infty, \infty)$. It is specified that $\theta \in (0^\circ, 180^\circ)$, with reflective boundary conditions, although flow speed variations associated

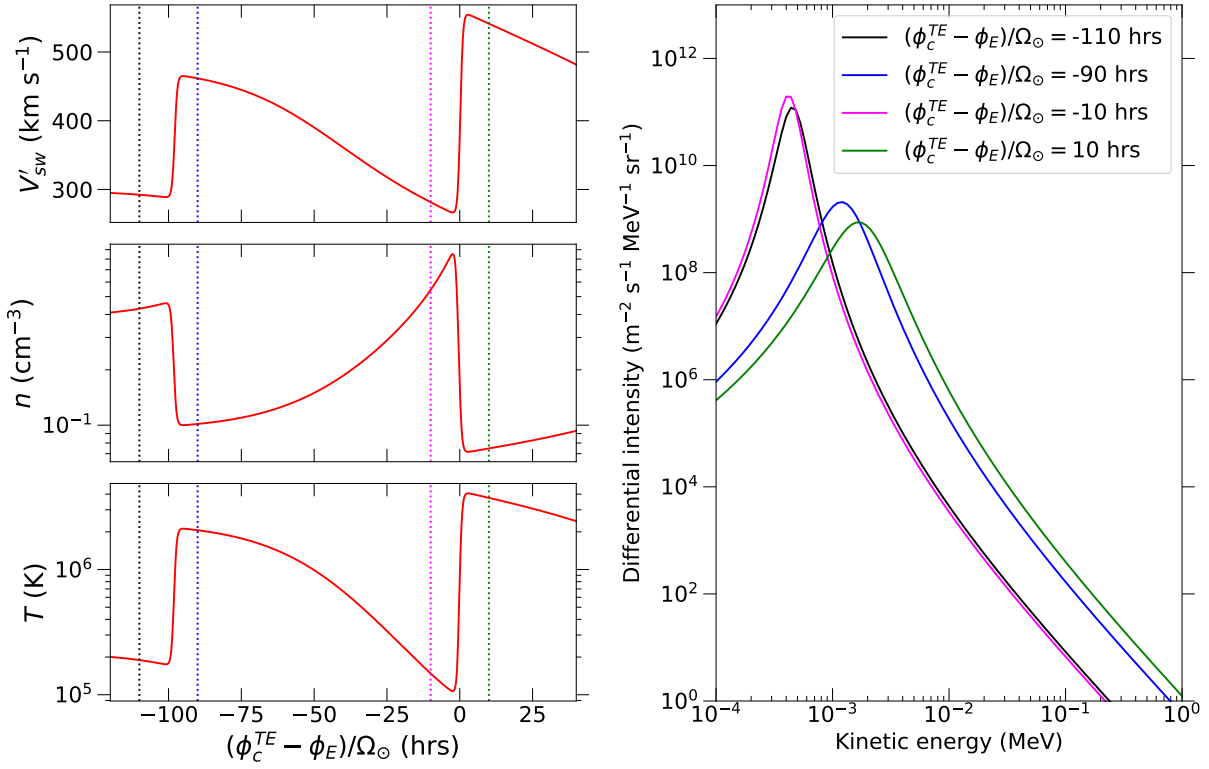


Figure 6.6: Similar to Figure 6.5, but shown for observer C as defined in Figure 6.1 at the coordinates $r_{\text{obs}} = 4$ AU and $\phi_{\text{obs}} = -180^\circ$.

with CIRs only extend up to $\sim 40^\circ$ away from the equatorial plane [e.g. Heber *et al.*, 1999], and particles transported to observers in this plane are shown in Section 6.5 to traverse an even smaller range in θ . While most other model attributes introduced in Section 5.2 are retained, changes involving the diffusion coefficients, time progression, injection energies, and magnetic field are discussed below.

6.3.1 Defining the simulation time

In Chapters 4 and 5 the simulation time is defined as the transit time of the CME-driven shock between the Sun and the Earth. To similarly define a time progression for CIR passages is more arbitrary. With the specific aim of studying particle acceleration, simulation times should be limited to avoid modulation processes concealing acceleration features. As such, the CIR is allowed to rotate through an angle

$$\Omega_\odot t_T = \phi_{c,f}^{LE} - \phi_{c,0}^{LE}, \quad (6.4)$$

where $\Omega_\odot$ is the corotation rate and t_T the total simulation time. The angles $\phi_{c,f}^{LE}$ and $\phi_{c,0}^{LE}$ represent the final and initial ϕ -positions of the leading edge compression as defined for Eq. 6.1. These parameters are chosen to simulate a single passage of the CIR structure past a set of virtual spacecraft, or observers, such as those shown in Figure 6.7. The spatial coordinates of these observers $(r_{\text{obs}}, \theta_{\text{obs}}, \phi_{\text{obs}})$ along with E_{obs} define the observational point for which the SDE solution is sought. As explained in the discussion of Eq. 6.1 in Section 6.2, the progression

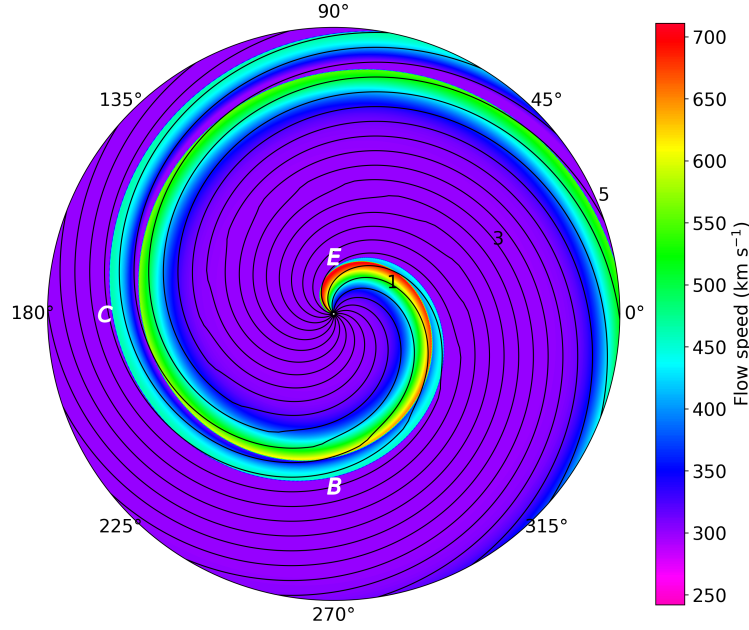


Figure 6.7: Similar to Figure 6.1 with corresponding projections of magnetic field lines onto the heliographic equatorial plane. In addition to the previously defined observers, the observer B is located at coordinates $(r, \phi) = (3 \text{ AU}, -90^\circ)$.

of the leading edge compression, to which other CIR parameters are coupled, defines the time progression in the model. Therefore, in a time-backward fashion, it follows that

$$\phi_c^{LE} = \phi_{c,f}^{LE} - \Omega_\odot t, \quad (6.5)$$

where $0 < t < t_T$. The position of the CIR is therefore updated in step with r , ϕ , θ , and E according to the SDEs in Eq. 3.27 (or Eq. 5.3, where relevant), where the time is once again incremented variably depending on the dominant radial transport process. In this configuration, the time at which $\phi_c^{LE} = \phi_{c,f}^{LE}$ gives the instant $t = t_{\text{obs}}$ during the CIR passage at which the distribution function at the observational point is sought.

Recall from Section 4.4.2 that the total simulation time influences how far the resultant shock-accelerated spectrum extends in energy. The termination of the spectrum is therefore implied to depend on the choice of $\phi_{c,0}$, where the spectrum extends to higher energies for smaller values of $\phi_{c,0}$. However, this effect is offset should the initial position of the CIR be specified further away from the observer, because the source of accelerated particles is also further removed. The solution obtained should therefore be approximately time-stationary for as long as $\phi_{c,0}$ is specified such that the observer is ahead of the CIR at $t = t_T$, where t_T is as defined in Eq. 6.4.

6.3.2 Modified scattering properties

With regards to the diffusion coefficients, the configuration applied here expands upon that introduced in Section 5.2. The characterizations of $\kappa_{\parallel}$ and $\kappa_{\perp r}$ remain unchanged, that is, $\kappa_{\parallel} \propto R^{1/3}$, while $\kappa_{\perp r}$ is approximated to be independent of rigidity and 2% of the magnitude of $\kappa_{\parallel}$. However, because acceleration is considered at CIRs beyond 1 AU, and to account for lower levels of magnetic turbulence further away from the Sun, MFPs are specified to increase with

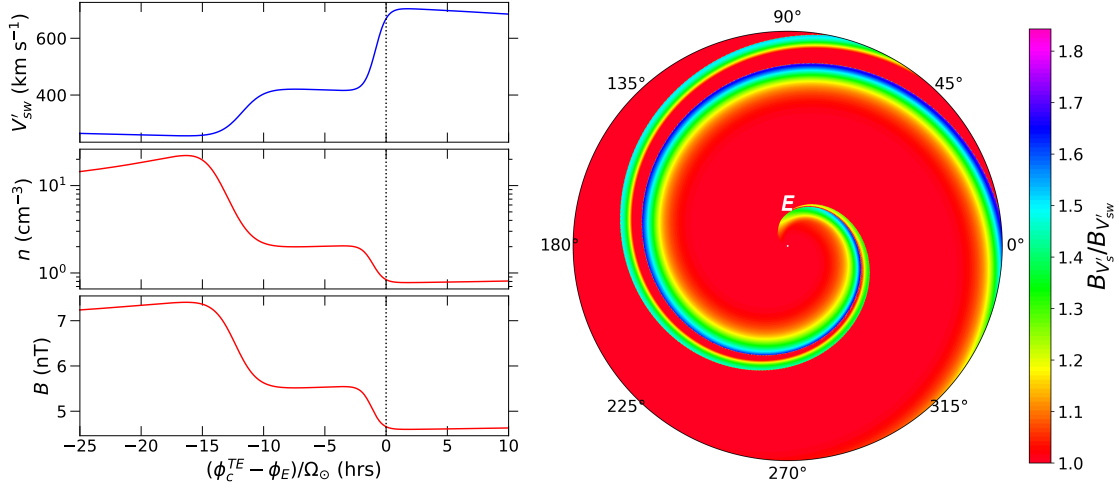


Figure 6.8: Left: Similar to the left panel of Figure 6.5 for an observer at Earth, but also including the evolution of the magnetic field magnitude during the CIR passage. The vertical line indicates the approximate position of the leading edge. Right: Magnetic compression ratios calculated from the magnetic field magnitudes associated with the slow SW flow speed V'_s and the CIR-associated flow speed V'_{sw} of Eq. 6.1. The E marker shows the observer for which the profiles on the left are given.

heliocentric distance [e.g. Engelbrecht and Burger, 2013]. Eq. 4.3 is accordingly modified as

$$\lambda = \lambda_0 \left(1 + \frac{r}{r_0}\right) \left(\frac{R}{R_0}\right)^{1/3}, \quad (6.6)$$

where, similar to previous chapters, λ_0 is chosen to yield an effective radial MFP of ~ 0.06 AU near Earth [$r_0 = 1$ AU Palmer, 1982]. Whereas the $(1 + r)$ factor gives the desired dependence beyond 1 AU, it is weaker for $r < 1$ AU, which simulates to some extent the radial independence of MFPs reported by Kallenrode et al. [1992] for diffusive SEP events at small heliocentric distances.

This radial dependence also replicates the effect that shock steepening would have on particle acceleration, despite the steepening process not being self-consistently included in Eq. 6.1. By virtue of the radially increasing diffusion length scales following from Eq. 6.6, particles sample greater fractions of the compression ratios of compression waves bounding CIRs at increasing distances from the Sun, even though the compression widths themselves are not specified to vary with radial distance. That is, in the limit where $\kappa_{rr}/V'_{sw} \gg \Delta_c$, where $\Delta_c = W_{ave}\Delta\phi_c/\Omega_\odot$ gives the thickness of the compression wave along the radial direction, the results of DSA are recovered [see also Drury, 1983; Jokipii et al., 2001; Giacalone et al., 2002]. Note that this limit generally applies in this study, since $\Delta_c \approx 0.005$ AU $< \kappa_{rr}/V'_{sw}$ for $\Delta\phi_c^{LE} = \Delta\phi_c^{TE} = 0.5^\circ$. Note furthermore that while cosmic ray modulation studies often decrease diffusion coefficients inside CIRs to simulate modulating barriers [e.g. Kota and Jokipii, 1991; Vogt et al., 2015], this is not an objective of the current study. Diffusion coefficients are therefore not scaled inside CIRs.

Where cross-field particle transport is concerned, axis-symmetrical turbulence is assumed, implying that $\kappa_{\perp\theta} = \kappa_{\perp r}$. The perpendicular diffusion governed by $\kappa_{\perp\theta}$ is relevant where transport out of the equatorial plane is considered (e.g. Section 6.5), however, as Section 5.5.3 illustrates, parallel diffusion along magnetic field lines with significant polar components, or latitude-dependent turbulence, would contribute more in this regard. However, cross-field dif-

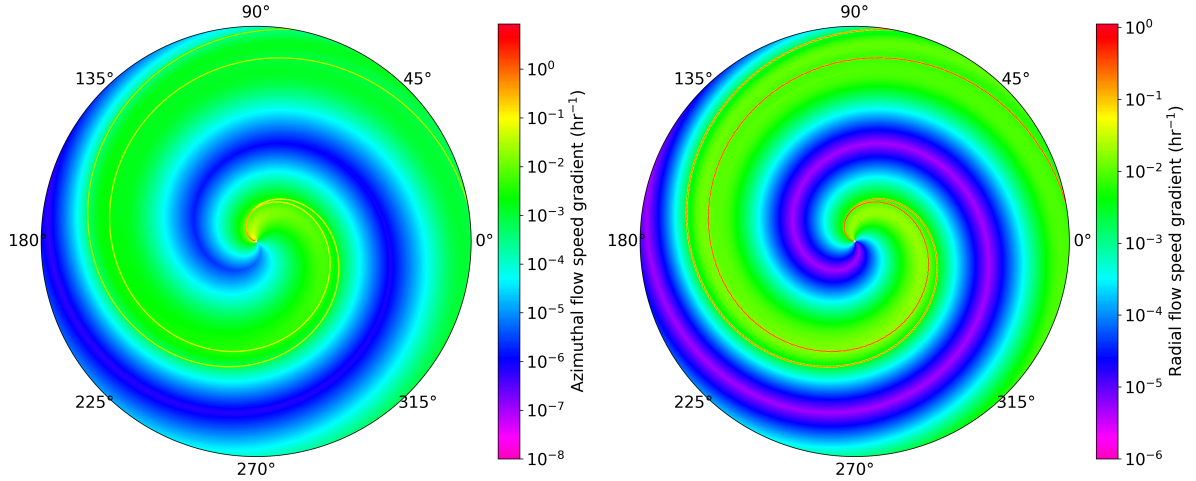


Figure 6.9: Spatial arrangements of the components of the flow speed gradient calculated from Eq. 6.1 in spherical coordinates. Left: The azimuthal flow speed gradients on which the magnetic field modification of Eq. 5.14 depends. Right: The radial flow speed gradients used to define the spatial extent of the source function in Eq. 4.11.

fusion may play an important role in providing seed particles for shock acceleration elsewhere along an extended CIR structure, since it provides a transport mechanism for particles from remote acceleration sites that are not magnetically connected to an observer.

6.3.3 Simulated CIR magnetic field properties

Particle transport is largely dependent on the form of the diffusion tensor, which in turn depends on magnetic field geometry. The projections of field lines onto the heliographic equatorial plane are illustrated in Figure 6.7 for the same configuration used in Figure 6.1. The field lines are coiled less inside the CIR where flow speeds are enhanced, but generally trace out the same spiral form as the CIR itself, as a result of corotation. As previously stated in this description, field lines from different plasma regimes may interpenetrate and could therefore intersect the SI. This analytical CIR description is optimized for investigating acceleration at the bounding compression waves (or shocks), but is not suitable for studying particles streaming along field lines at *e.g.* the SI. Focused transport models paired with MHD simulations are more appropriate in this regard [*e.g.* [Wijsen et al., 2019](#)].

In terms of magnitudes, the combined description of Eqs 6.1 and 5.16 provides reasonable reproductions of magnetic properties inside CIRs. As the left panel of Figure 6.8 shows, the magnetic field inside the CIR scales in a similar manner to the density from the perspective of an observer at Earth, and both these quantities show enhancements associated with regions with positive flow speed gradients [see *e.g.* [Belcher and Davis, 1971](#)]. The right panel of Figure 6.8 illustrates by which factor the magnetic field in the uncompressed slow SW is larger than inside the CIR. Illustrated in this way, the CIR structure is clearly visible, and the otherwise dominating radial components are suppressed. Magnetic fields inside the interaction region are the smallest just behind the compressions at the leading and trailing edges of the CIR, with those behind the latter being smaller for the current configuration. From there the magnetic fields gradually recover in the rarefaction region along the inner edge of the CIR.

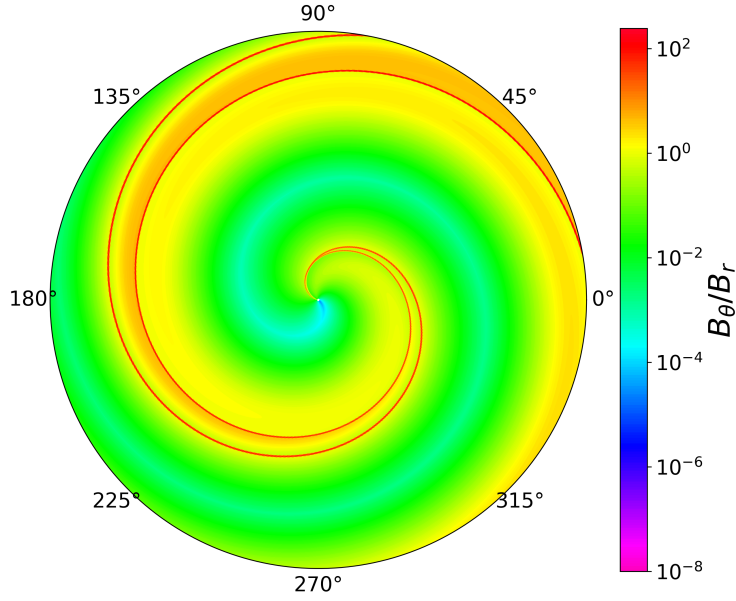


Figure 6.10: An illustration of the magnetic field modification to the *Parker* [1958] spiral (also the θ -component of the modified field) calculated from Eq. 5.14 as a ratio of the radial magnetic field component. This plot corresponds to the flow speed configuration in Figure 6.7.

In contrast to the simple 2D CME geometry introduced in Section 5.3, the azimuthal gradient of V'_{sw} of Eq. 6.1 is both larger and distributed more widely, as shown in the left panel of Figure 6.9. Consequently, the magnetic field modification of Eq. 5.14 is also more globally prominent. This is illustrated in Figure 6.10 for the heliographic equatorial plane. As expected, B_θ is large near, and especially inside, the CIR, while decreasing further away from it. The largest gradients and θ -components in the magnetic field are evident at the leading and trailing edge compression waves. The correct interpretation of the magnetic field modification should be borne in mind: these enhanced polar components simply measure the compensation required for magnetic fields associated with local flow properties to remain divergence free. They do not necessarily follow as any physical consequence of the flow properties inside the CIR. Nevertheless, these large polar components imply that particles can be transported out of the equatorial plane efficiently by means of parallel diffusion. This is investigated in Section 6.5.

6.3.4 A spatial injection model for CIR particle acceleration

Figure 6.7 shows magnetic field lines intersecting the CIR at varying angles. At small heliocentric distances, field lines tend to intersect the CIR at larger angles relative to the compression wave front (or smaller angles relative to its normal) than further along the CIR. Similar to parallel shocks, a lower energy threshold may be required for particles to return to the compression wave front if the magnetic field intersecting it is nearly normal to its surface [*Giacalone et al.*, 1992; *Neergaard-Parker and Zank*, 2012]. Given the high spatial variability in the obliquity of corotating compression waves, a variable injection energy, based on the relative geometries of the CIR and magnetic field, is implemented.

Firstly, consider a CIR in the heliographic equatorial plane and a *Parker* [1958] magnetic field ($B_\theta = 0$). An angle Ψ separating $\vec{B}$ from the radial direction is sought, which in this case is the

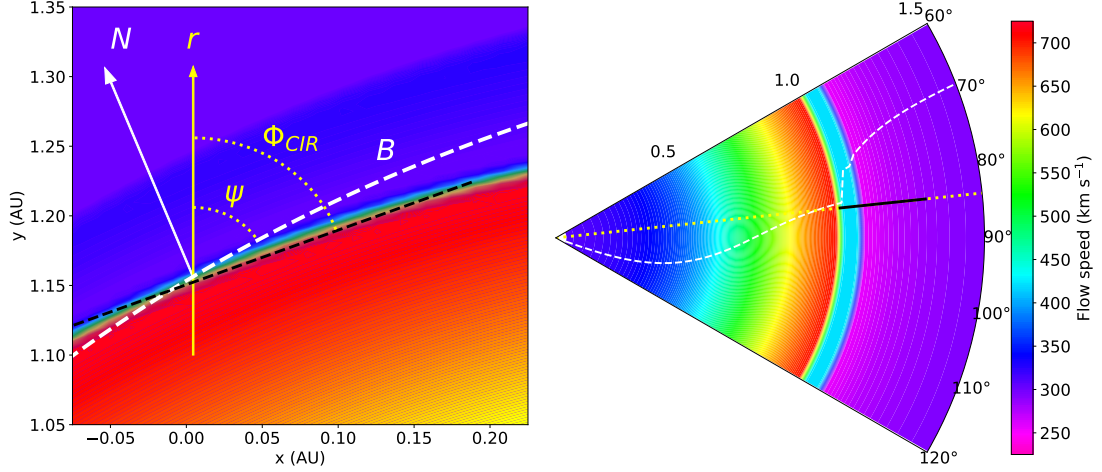


Figure 6.11: Left: Schematic of the magnetic field line geometry at the intersection with an edge of the CIR. Here, the dashed white line labeled B represents a magnetic field line, whereas the solid white line labeled N gives the vector normal to the compression wave front. The angles Ψ and Φ_{CIR} , as defined by Eqs 6.7 and 6.8, give the respective angles separating the magnetic field and the wave front from the radial direction. Right: A meridional cross-section of the CIR, where the solid black line indicates the normal of the compression wave at the trailing edge in the (r, ϕ) -plane. The dashed white line is a sample magnetic field line.

magnetic winding angle ψ calculated from the ratio of the azimuthal and radial components. That is,

$$\Psi = \psi = \tan^{-1} \left(\frac{\Omega(r - r_{\odot}) \sin \theta}{V'_{sw}} \right), \quad (6.7)$$

where ψ is as defined for Eq. 5.1. By analogy, an angle separating a tangent on the corotating compression wave front from the radial direction is similarly defined as

$$\Phi_{\text{CIR}} = \tan^{-1} \left(\frac{\Omega(r - r_{\odot}) \sin \theta}{W_{ave}} \right), \quad (6.8)$$

where $\Omega(r - r_{\odot}) \sin \theta$ is the component of the compression wave front dragged out along the azimuthal direction as a result of corotation, and W_{ave} is the radial speed of the CIR as defined in Eq. 6.3. These angles are illustrated schematically in Figure 6.11. Obliquity, however, concerns the orientation of the magnetic field relative to the normal of the compression wave. From Figure 6.11, this angle is given by

$$\begin{aligned} \Theta_{\text{BN}} &= \begin{cases} 90^\circ - (\Phi_{\text{CIR}} - \Psi) & \Phi_{\text{CIR}} > \Psi \\ 90^\circ + (\Phi_{\text{CIR}} - \Psi) & \Phi_{\text{CIR}} < \Psi \end{cases} \\ &= 90^\circ - |\Phi_{\text{CIR}} - \Psi|. \end{aligned} \quad (6.9)$$

Suppose furthermore that a particle travelling along a field line is incident on the compression wave at a speed of v_{inj} . If the upstream flow speed in the frame of the compression wave and projected onto the normal of the compression wave is given by $|V'_S - W_{ave}| \sin \Phi_{\text{CIR}}$, the minimum speed required for particles to return to the compression wave front follows as

$$v_{\text{inj}} = \frac{|V'_S - W_{ave}| \sin \Phi_{\text{CIR}}}{\cos \Theta_{\text{BN}}}, \quad (6.10)$$

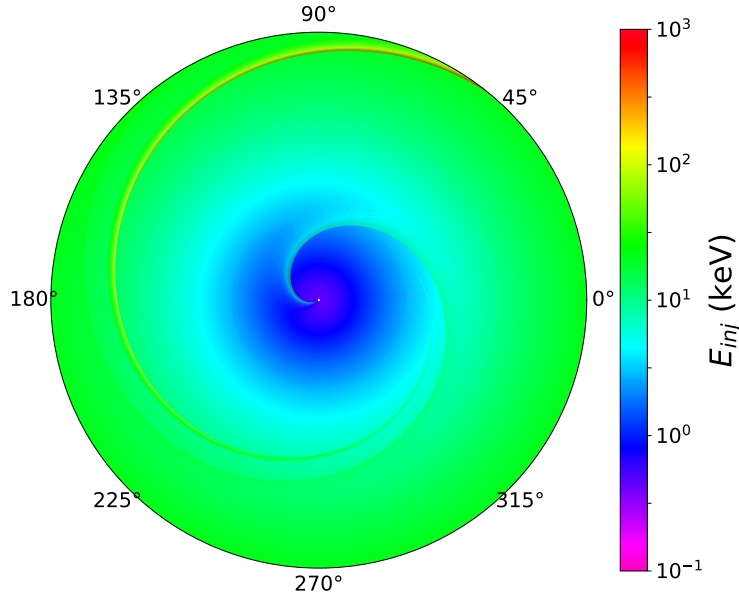


Figure 6.12: Spatial dependence of the injection energies calculated from Eqs 6.10 and 6.11 for CIR compression waves for the same flow speed configuration in Figure 6.7.

from which the injection energy can be calculated using

$$E_{\text{inj}} = m_p c^2 \left(\frac{1}{\sqrt{1 - (v_{\text{inj}}/c)^2}} - 1 \right). \quad (6.11)$$

The resulting injection energies for a CIR in the heliographic equatorial plane are illustrated in Figure 6.12. Of course, the injection energies shown here are only meaningful near the CIR. As such, they are best viewed in conjunction with the radial flow speed gradients in Figure 6.9, because $\partial V'_{sw}/\partial r$ is representative of the source region as defined in Eq. 4.11. The injection energies range from ~ 1 keV at small heliocentric distances to several hundred keV at larger distances along the CIR, which suggests that the obliquity of the compression waves bounding the CIR transitions from quasi-parallel to quasi-perpendicular with increasing distance. The injection threshold is especially high ahead of the reverse compression at larger heliocentric distances. Note however that the assumption of laminar magnetic field lines likely contributes to the strong radial dependence of E_{inj} shown in Figure 6.12. This dependence may be relaxed with the inclusion of a turbulent magnetic field. The mean injection energy appears to be of the order of 10 keV.

In the 3D description, ψ measures the angular separation between $\vec{B}$ and the meridional (r, θ) plane, whereas the above derivation requires the angle between the projection of $\vec{B}$ onto the (r, ϕ) -plane and the radial direction. Eq. 6.7 is therefore replaced in the 3D description by

$$\Psi = \tan^{-1} \left(\frac{\tan \psi}{\cos \zeta} \right), \quad (6.12)$$

where ψ and ζ are as defined for the diffusion tensor elements in Eq. 3.22 [see also *Burger et al.*, 2008]. Moreover, because V'_{sw} is specified in Eq. 6.1 as a function of only r and ϕ , and is essentially symmetrical across the heliographic equatorial plane, the normal of the corotating

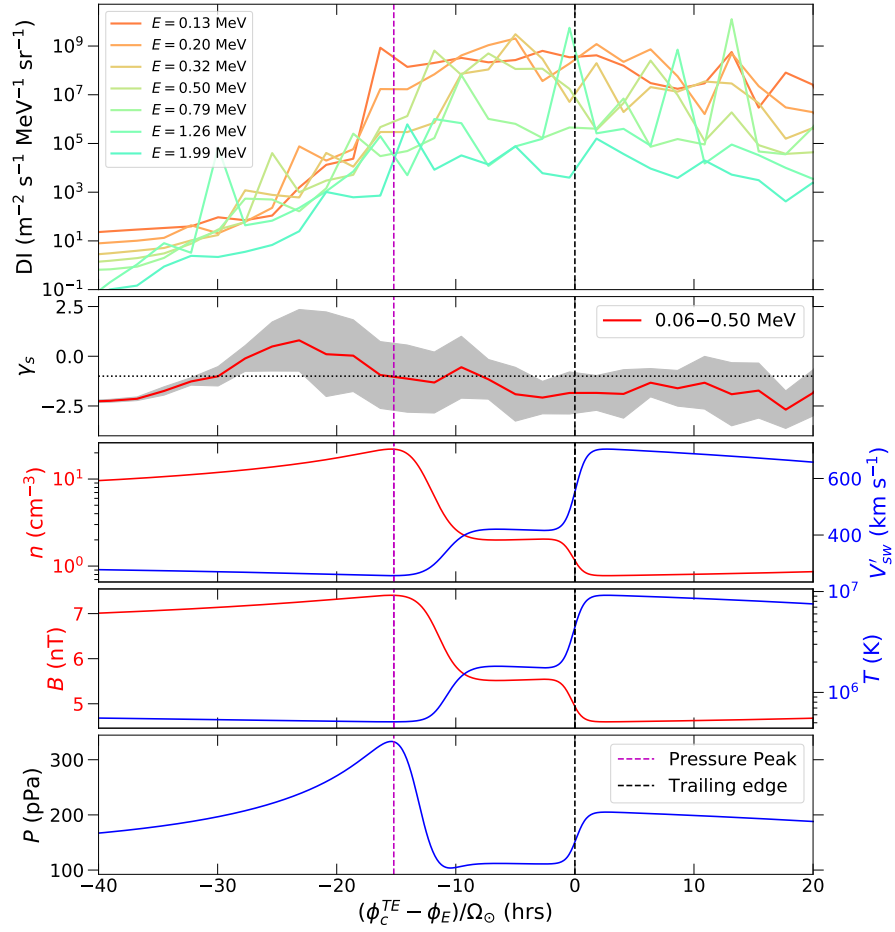


Figure 6.13: Simulated intensities of energetic protons accelerated from the suprathermal SW during the passage of a CIR at Earth. The top panel shows simulated particles intensities for different energies between ~ 0.1 and 2 MeV. The second panel gives the average spectral index γ_s of the simulated energy spectrum between 60 and 500 keV as a function of time. Here, the shaded area indicates the standard deviation, and the horizontal line a spectral index of -1 . The SW quantities correspond to those given in Figures 6.5 and 6.8, while the total SW proton pressure is calculated from these as $P = 2nk_B T + B^2/2\mu_0$. The vertical lines in black and magenta give the approximate locations of the CIR trailing edge and pressure peak, respectively.

compression wave is assumed to have no θ -component. Eq. 6.8 therefore remains unchanged from the 2D description.

6.4 Features of CIR particle acceleration: reference solutions

The acceleration of particles at compression waves associated with CIRs is simulated for three spatial dimensions, as discussed in Section 6.3. The description of the SW and the energy distribution of SW particles, which serve as seed particles for acceleration, is implemented as discussed in Section 6.2. Simulated particle intensity profiles are presented in Figures 6.13 and 6.14 for observers E and C of Figure 6.7. They are accompanied by simulated time profiles of the SW flow speed V'_{sw} , number density n , temperature T , magnetic field magnitude B , and the total SW proton pressure, given by $P = 2nk_B T + B^2/2\mu_0$, where k_B and μ_0 are the Boltzmann constant and permeability of free space, respectively. Similar quantities are presented by *e.g.*

Ebert et al. [2012] for the analyses of ACE and STEREO A & B observations for the proximity of intensity peaks relative to CIR trailing edges and pressure peaks.

In Figure 6.13, for an observer at Earth, the simulated SW plasma profiles provide comparable qualitative descriptions for their counterparts in observations, *e.g.* those presented by *Ebert et al.* [2012]. For example, the magnetic field magnitude and number densities similarly show enhancements ahead of the SI. As a result, the pressure peaks at a similar position within the compressed slow SW. The simulated intensities of particles accelerated throughout the interaction region reproduce the most noticeable features of intensity-time profiles in observations [*e.g.* *Richardson and Zwickl*, 1984; *Chottoo et al.*, 2000; *Bučík et al.*, 2009; *Ebert et al.*, 2012]. Intensities are enhanced within the interaction region, with an abrupt onset relative to the more gradual decline of intensities following the passage of the trailing edge. The intensity enhancements for low-energy particles are typically larger than for high-energy particles, which is suggestive of the involvement of DSA, which tends to arrange intensities according to a power law decreasing with energy.

To aid in this analysis, the evolution of the average spectral index γ_s of the energy spectrum between 60 and 500 keV is also shown in Figure 6.13, along with error margins that scale roughly according to the levels of stochastic variation in the particle intensities. The spectral indices associated with the local compression ratios at either end of the interaction region are included within these error margins. For example, at the trailing edge, $\gamma_s \approx -2$, which DSA theory predicts would follow from a compression ratio of 2. Indeed, the number density decreases across the trailing edge by a similar factor. The change in number density from the unperturbed slow SW to within the interaction region is roughly a factor of 4 if the density enhancement ahead of the SI is disregarded. The spectral index in this region is $\gamma_s \approx -1$, which is associated with a strong shock with a compression ratio of at least 4.

It should be cautioned, however, that because the SW velocity divergence is non-zero and negative throughout the interaction region, particles may sample various compression sizes. In addition to DSA at the bounding compressions, particles can gain energy by being scattered either across the whole SIR (in the case of high-energy particles with large MFPs) or within them, *e.g.* according to the mechanism proposed by *Giacalone et al.* [2002]. The spectral indices may therefore not necessarily reflect local compression ratios. Note that the trailing edge spectra are usually considered to be harder than at the leading edge, even at Earth [*Fisk and Lee*, 1980]. In this case, if local compression ratios at Earth are larger for the leading edge than for the trailing edge, but with harder spectra at the latter, it is possible that particles are transported there from a magnetically connected reverse shock elsewhere along the trailing edge [*Scholer et al.*, 1999]. Another consideration is that of modulation effects, which also influence the form of energy spectra. Particle intensities in Figure 6.5 show little variation with energy at the onset of the intensity enhancements. The corresponding spectral indices are also roughly zero, which is indicative of spectral flattening and likely a result of modulation owing to rigidity-dependent diffusion or adiabatic energy losses, similar to what is seen ahead of ESP events as discussed in Section 4.6.2.

For observer C in Figure 6.6, two distinguishable intensity enhancements are visible around the leading and trailing edges, respectively, with the intensities around the latter being sig-

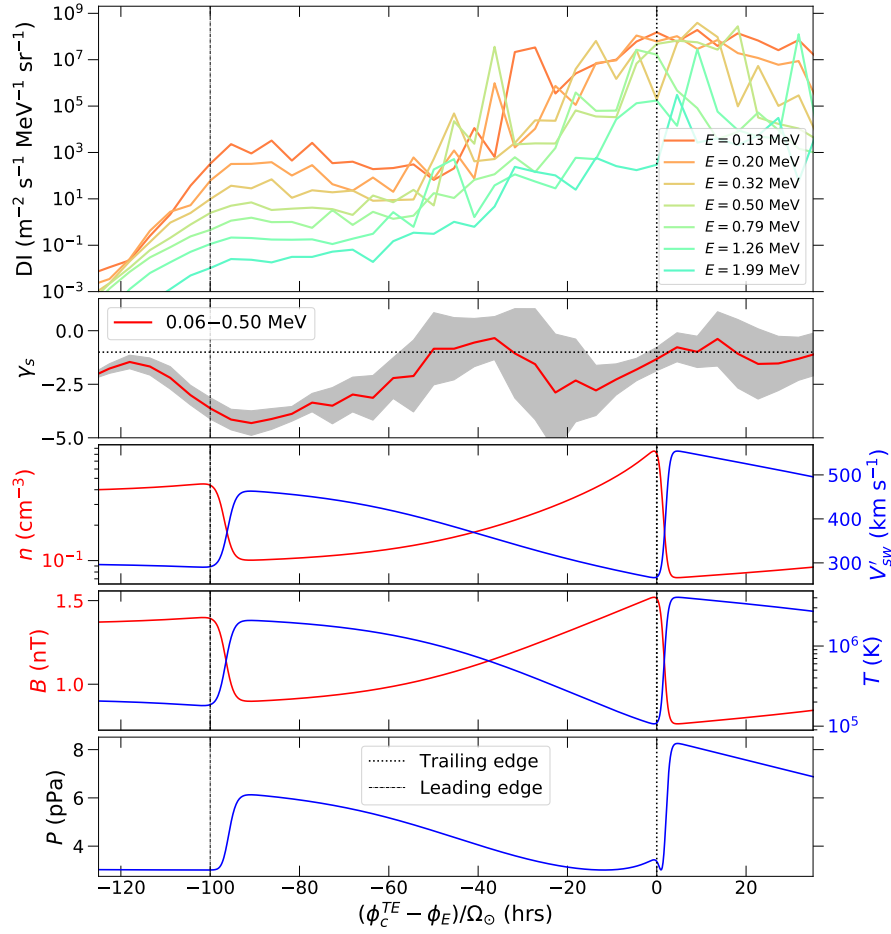


Figure 6.14: Similar to Figure 6.24, but for observer C (of Figure 6.7) at $r_{\text{obs}} = 4$ AU and $\phi_{\text{obs}} = -180^\circ$. Here, the SW quantities correspond to those in Figure 6.6. The dashed and dotted vertical lines give the approximate positions of the leading and trailing CIR edges, respectively.

nificantly higher. As before, spectral indices associated with the onsets are enhanced. Large spectral flattening occurs roughly 40 hours ahead of the arrival of the trailing edge, probably owing to the modulation of particles as they propagate from their acceleration site at the trailing edge toward the observer. This effect is noticeable ahead of the leading edge as well, although to a lesser degree. The higher energy particles are noticeably less modulated here, and their intensities seem to approach that of the κ -functions from which they are injected. If acceleration within a particular energy range is inefficient, spectra may retain their source spectral forms [Axford, 1981]. Moreover, whereas the spectral indices near the trailing edge reflect those predicted by DSA for a strong shock, those at the leading edge are conspicuously small. This follows because at the leading edge the energy spectrum in the 60 – 500 keV range is already in the exponential decrease phase. This is illustrated in Section 6.6.1.

With regards to peak intensities, the highest intensities in Figure 6.6, that is, as viewed by an observer at 4 AU, occur near the trailing edge [see also Desai *et al.*, 1998]. It is unclear from Figure 6.5, for an observer at Earth, whether the intensities definitively peak near the trailing edge, since especially low-energy particle intensities also appear enhanced near the pressure peak. The discussion of the organization and dependence of peak intensities associated with CIR particle acceleration continues in Section 6.6.

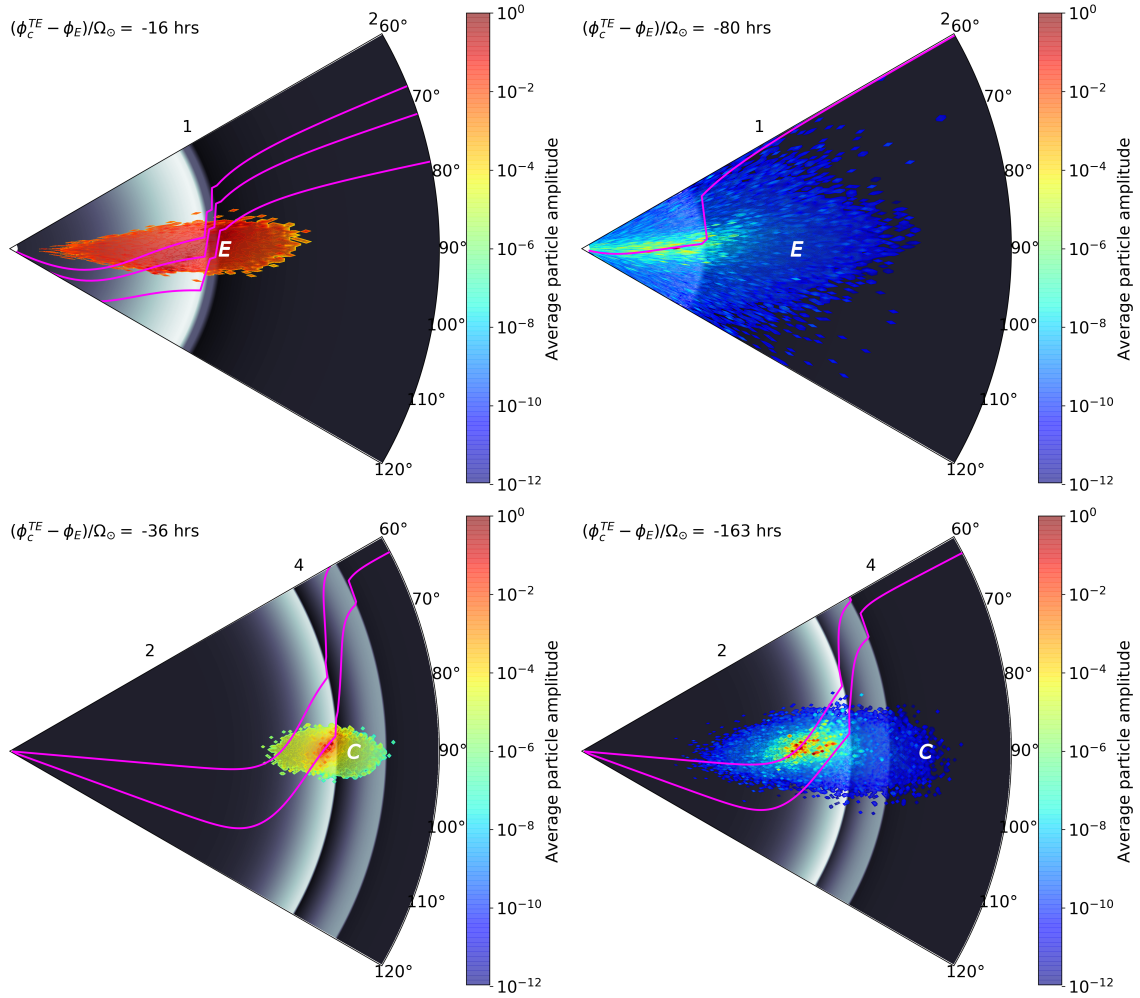


Figure 6.15: Prior distributions of CIR particles contributing to 500 keV intensities during the CIR trailing edge passage at each of the observers E and C as shown in the top and bottom panels, respectively. Similar to Figure 4.18, the color scale indicates the average particle amplitudes at each point in the meridional plane of the observer, where the maximum amplitude has been normalised to unity. These distributions are shown for the indicated times prior to the CIR trailing edge arrival. The corresponding flow speeds are given in a monochromatic scale in the background. The magenta lines are projections of sample magnetic field lines.

6.5 Trans-equatorial transport of CIR particles

This study is primarily concerned with the intensities of CIR particles as viewed by observers in the heliographic equatorial plane. The inclusion of the polar magnetic field component to ensure a divergence-free field (Section 5.4) necessitates the implementation of the diffusion tensor of Eq. 3.22 for a 3D field-line geometry. Although particles are also transported into and out of the equatorial plane by perpendicular diffusion, this transport is significantly enhanced should the magnetic field gain a large θ -component, because $\kappa_{\parallel} \gg \kappa_{\perp\theta}$ as illustrated in Section 5.5.3. This section investigates how the inclusion of B_θ affects particle intensities in the equatorial plane, and evaluates whether solving the 2D TPE provides adequate approximations.

As Figure 6.10 illustrates, the magnetic field correction is larger nearer to the CIR and particularly at the compression waves bounding it. This implies greater poleward contortion of field lines within these regions and is illustrated in Figure 6.15. These plots map the earlier distri-

butions of particles contributing to 500 keV intensities as viewed by the observers E and C at the moment of the trailing edge's arrival. The accompanying monochromatic plots of the flow speeds are given in the meridional (r, θ) plane of each observer, while the field lines are projections onto this plane. Although the particle distributions are averaged over ϕ , their azimuthal positions along the CIR spiral structure can still be inferred from their radial positions.

There are a number of notable features from Figure 6.15 to discuss. Note firstly that the distributions of the most significantly contributing particles tend to follow the position of the compression wave at the trailing edge. These distributions also become more compact nearer to the arrival of the trailing edge. Taken together, these features imply that particles observed during the CIR passage are predominantly accelerated locally. It is furthermore apparent that the highest particle amplitudes are distributed along field lines, suggesting that parallel diffusion is indeed the dominant transport process. By contrast, the distribution of particles transported to the observer by perpendicular diffusion is much more sparse, as illustrated in the bottom-right panel of Figure 6.15. Despite significant diffusion along field lines with large B_θ -components, these earlier particle distributions show a limited and near-symmetrical spread in the θ -coordinate, extending no more than $\sim 5^\circ$ on either side of the equatorial plane. The CIR structure itself is symmetrical across the equatorial plane, which may further contribute to largely θ -independent transport. In this configuration, most particles contributing to intensities observed in the equatorial plane are therefore transported to the observer without meaningful excursions out of this plane. This implies, in turn, that solving the TPE limited to transport in only two spatial dimensions relative to the classic *Parker* [1958] magnetic field may yield results that are comparable to the 3D description.

Sample solutions of both the 2D and 3D descriptions are shown in Figure 6.16, attained by solving the SDEs of Eqs 5.3 and 3.27, respectively. Compared here are the time profiles of 100 keV, 500 keV, and 1 MeV particle intensities as viewed by observers E and C, along with the simulated energy spectra observed by each during the passage of the trailing edge of the CIR. Both sets of solutions display the properties discussed in Section 6.4: a steep onset of intensity enhancements relative to a more gradual decline, and power-law distributed energy spectra that terminate above particular cut-off energies. While it appears as if the 3D solutions undershoot the 2D solutions in some cases, the two sets of solutions are generally comparable within the margins of stochastic variation. Note that the 2D and 3D descriptions may not produce such similar results if the observational points are specified further away from the equatorial plane; however, such cases are not considered in the current study. Given the relative equivalence of the above solutions, and the limited symmetrical distribution of contributing particles about the equatorial plane, the 2D solutions serve as serviceable approximations when considering particle transport in or near the equatorial plane.

The solution of a third spatial SDE, including the calculation of all accompanying coefficients involving θ , increases the total computation time by a significant amount. For example, to generate the solutions displayed in Figure 6.16, the average wall-clock time per pseudo particle required by the 3D model is 4.4 seconds as opposed to 0.5 seconds for the 2D model using the same number of computational threads. The 2D solutions are therefore generated faster by nearly an order of magnitude. This advantage is exploited in Section 6.6, where multiple sets

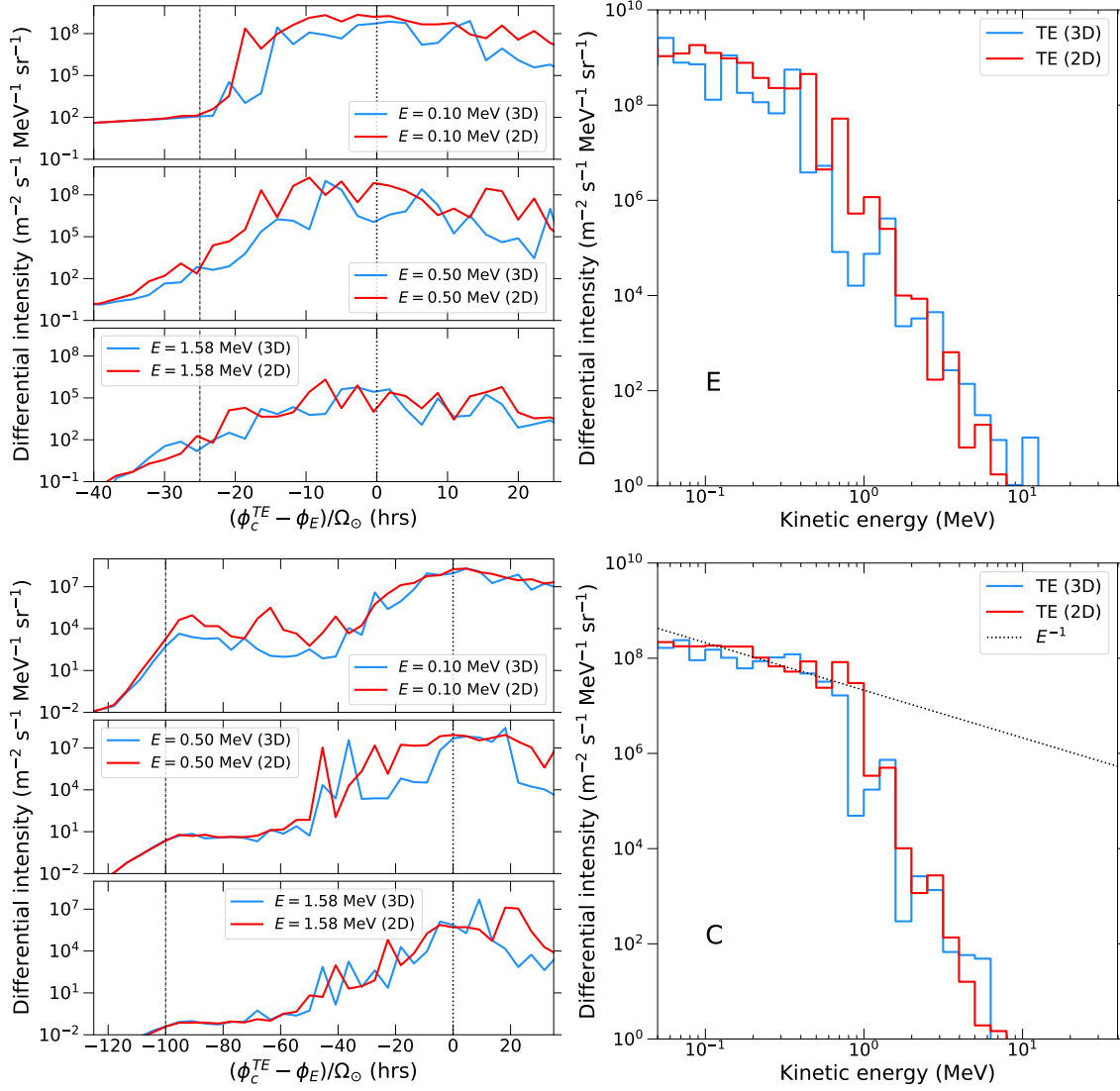


Figure 6.16: Comparisons of the solutions of the 2D and 3D TPEs of Eqs 5.2 and 3.23, as shown for observer E and C (of Figure 6.7) in the top and bottom panels, respectively. Left: Intensity-time profiles for the energies as shown in the legends. The dashed and dotted vertical lines represent the approximate positions of the leading and trailing CIR edges, respectively. Right: Energy spectra at the trailing edge of the CIR.

of SDE solutions are computed using the 2D approximation.

6.6 Organization of peak CIR particle intensities

Section 6.4 raised the question of where within the interaction region the intensities of particles accelerated there are expected to peak. Observations of CIR-associated suprathermal (~ 0.01 – 0.5 MeV) ions near 1 AU show intensities peaking in the compressed fast SW stream, between the SI and the trailing edge of the compression region, while higher-energy particle intensities may peak beyond the trailing edge in the fast stream [Chottoo *et al.*, 2000]. Ebert *et al.* [2012] also found that peak intensity times are better organized by the arrival time of the trailing edge rather than the pressure peak. The aforementioned studies relate these peak intensities to the trailing edge both in the presence and absence of a reverse shock at this boundary.

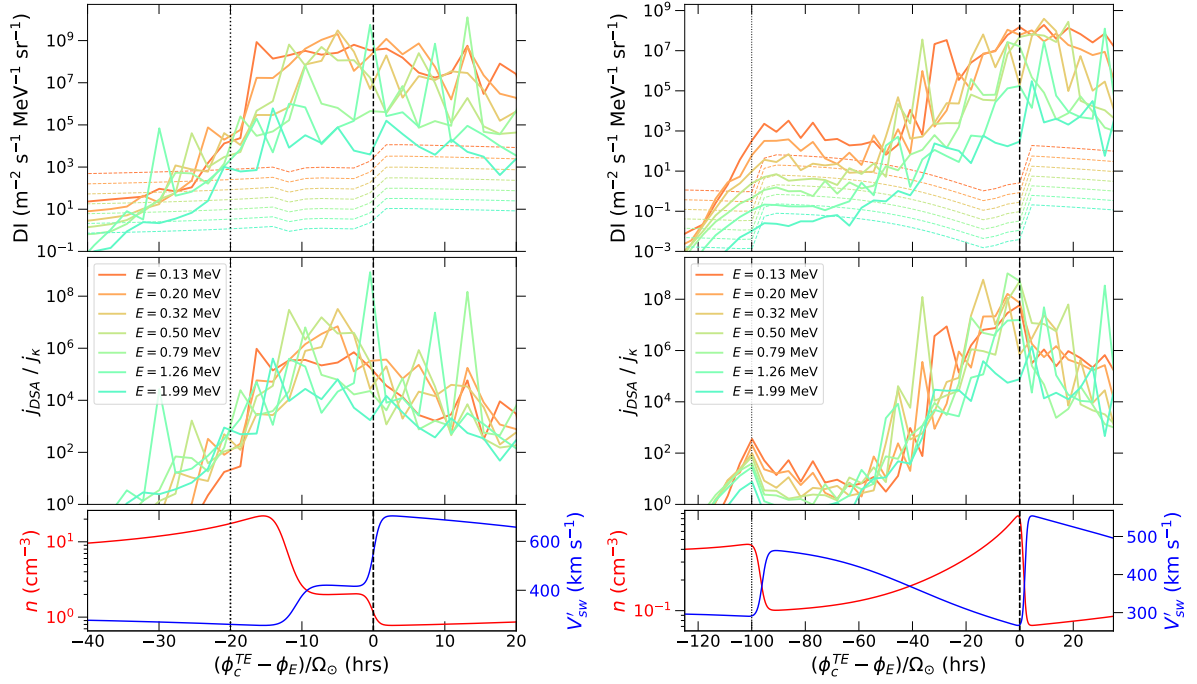


Figure 6.17: Top: Simulated intensities corresponding to those shown in Figures 6.13 and 6.14 for observers E and C, as shown on the left and right, respectively. Dotted lines in the same colours represent the corresponding profiles of the SW distribution as represented by the κ -function. Middle: Ratios of the intensities resulting from acceleration to those of the SW distribution for energies corresponding to the profiles above in similar colors. Bottom: The corresponding SW flow speeds and densities as given before. Dotted and dashed vertical lines indicate the positions of the CIR leading and trailing edges, respectively.

In an attempt to accentuate the positions of peak intensities in the simulated intensity profiles presented in Figures 6.13 and 6.14, the ratios of these intensities to those of the local SW distribution (represented by the κ -function) are calculated. These ratios give a measure of the efficiency of the acceleration process alone and factors out the contribution of the heated SW distribution to intensity enhancements. These are shown in Figure 6.17. For the observer at Earth, the ratios make it more apparent that intensities are generally still rising after the passage of the leading edge and pressure peak, and for most energies reach their maxima in the compressed fast stream within 10 hours before the arrival of the trailing edge (consistent with the findings of *Chottoo et al.* [2000] and *Ebert et al.* [2012]). Higher energy particles ($\gtrsim 1$ MeV) are more gradually enhanced across the interaction region at Earth, and show less definitive peaks (if any at all). This may be because high-energy particles have diffusion length scales that are larger relative to the interaction region. They may therefore sample a greater fraction of the flow speed changes across the compressed SW region, so that their intensity profiles do not necessarily reflect the properties of any substructure of the interaction region.

For the other observer further along the CIR, at 4 AU, intensities clearly reach a global maximum near the trailing edge [*Desai et al.*, 1998]. However, in this case, the jumps in SW quantities at this boundary are larger than at the opposite end of the interaction region. This is in contrast with the observer profile at Earth, where the density jump is smaller at the trailing edge. This draws the dependence of peak intensity positions and magnitudes on local compression ratios into question. These issues are addressed in the sections below.

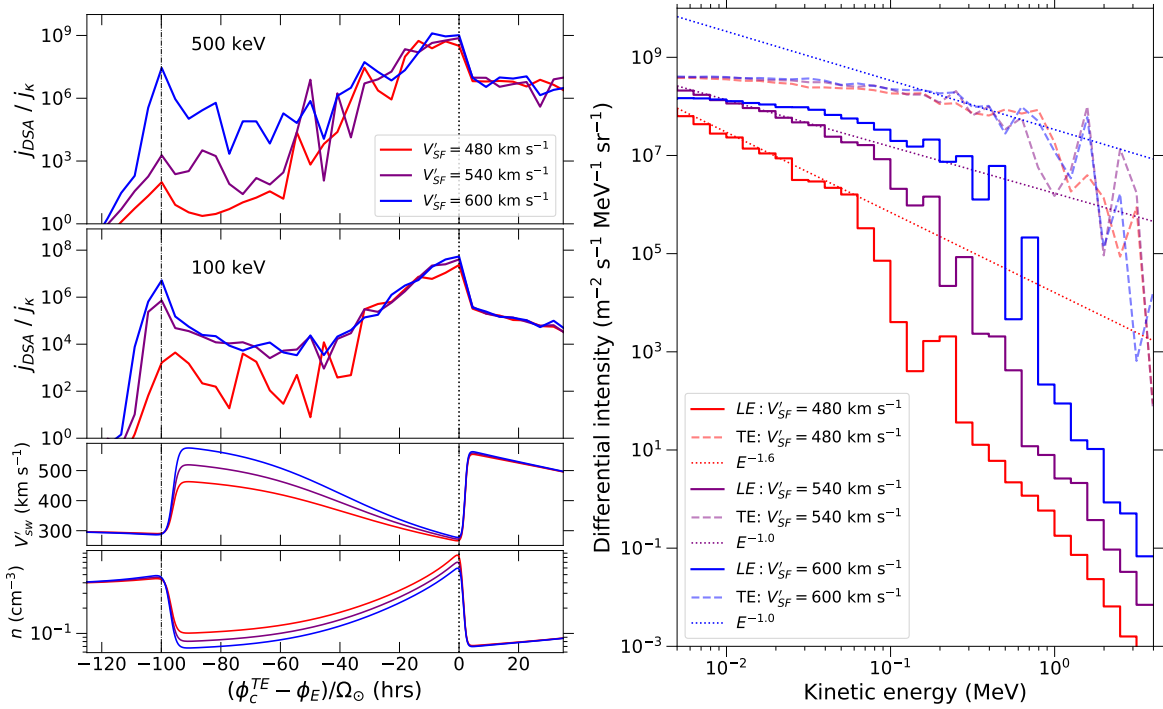


Figure 6.18: Left: Simulated intensity ratios for observer C (of Figure 6.7) similar to those shown in Figure 6.17, but only for 100 and 500 keV particles, and for varying values of V'_{SF} in Eq. 6.1 as indicated in the legend. The corresponding SW flow speeds and densities are given for ease of reference. The dashed and dotted vertical lines give the approximate positions of the leading and trailing CIR edges, respectively. Right: Simulated energy spectra for the same V'_{SF} -values varied on the left at both the leading and trailing edges of the CIR. Dotted lines are fits to the power-law segments of spectra with the spectral indices indicated in the legend.

6.6.1 Leading versus trailing edge acceleration

For observer C in Figure 6.17, the intensity enhancements are the largest at the trailing edge of the interaction region. These intensity enhancements are accompanied by large jumps in SW quantities, and in particular, the number density, according to which the spectral indices of shock-accelerated spectra scale (as extensively discussed in Chapter 4). Furthermore, reverse shocks, which are often encountered at the trailing edge at large heliocentric distances [Hundhausen and Gosling, 1976], are considered efficient accelerators [Lee and Fisk, 1982]. These factors should contribute toward large local intensity enhancements. However, the peak in the intensity profile for the observer at Earth does not accompany the larger density jump.

For comparison purposes, the factors by which the fixed-frame flow speeds jump across the leading edge of the interaction region, as viewed by observer C, is varied by scaling the parameter V'_{SF} in Eq. 6.1. The left panel of Figure 6.18 shows how this affects the time profiles of the ratios introduced for Figure 6.17. By increasing the flow speed ratio across the leading edge, the number density ratio also increases, until for $V'_{SF} = 600$ km/s, the number density jumps by approximately the same factor as seen at the trailing edge. For larger jumps across the leading edge, the intensity enhancement at this boundary becomes progressively larger. However, even in the case where the compression ratios across each boundary are comparable, the intensity enhancements are still larger at the trailing edge. Aside from compression ratios, there are other factors that could affect this outcome: firstly, intensities may be higher near the trail-

ing edge owing to the accumulation of particles from prior acceleration, both at the leading edge and throughout the interaction region by converging scattering centres in the SW [Giacalone *et al.*, 2002]. Related to this, the effect of corotation promotes particle transport toward the trailing edge during the passage of the interaction region. Consider furthermore that since flow speeds are enhanced in the fast stream beyond the trailing edge, diffusion length scales are smaller there. This improves confinement of particles at the trailing edge, impeding their escape into the fast stream, while corotation carries more particles toward this boundary from inside the interaction region. Together these factors create conditions that are highly conducive for DSA.

Figure 6.18 nonetheless shows that varying the compression ratio does affect the height of intensity peaks. How this occurs may be explained by considering the energy distributions of accelerated particles as shown in the right panel of Figure 6.18. Of course, increasing compression ratios results in harder shock-accelerated spectra, which disproportionately raises the intensities of higher energy particles. This is why the 500 keV ratios in Figure 6.18 appear more sensitive to varying V'_{SF} than the 100 keV ratios. For density jumps larger than 4, the spectral indices adopt a maximum value of -1 . Note the spectra for both $V'_{SF} = 540$ and 600 km s^{-1} are distributed along E^{-1} . However, the latter extends to higher energies. Recall from Section 4.4.2 that the energy up to which these power-law spectra extend is time-limited. Given that the same simulation times were allowed for the solutions shown in Figure 6.18, the factor limiting the cut-off energy is therefore related to the efficiency of acceleration within the available time. Particles gain more energy per crossing when being scattered across compression waves with larger compression ratios. For a fixed simulation time, this could explain why the spectrum for $V'_{SF} = 600 \text{ km s}^{-1}$, as well as the trailing edge spectra extends to higher energies.

Thus, in summary, the positions of peak intensities tend to be closer to the trailing edge owing to more efficient acceleration at this boundary because of the joint effects of corotation and smaller diffusion length scales in the adjacent fast stream. Moreover, a causal relationship is identified between peak intensities and local compression ratios. The following section explores this relationship quantitatively.

6.6.2 Correlations of peak intensities with local compression ratios

Ebert *et al.* [2012] found that when intensities peak in close proximity to the trailing edge, these peak intensities scale proportionally to local magnetic compression ratios, regardless of whether a reverse shock is present or not. Another study by Bučík *et al.* [2009] considers how these peak intensities scale with compression thickness and pressure peaks, respectively, finding an inverse correlation with the former and a direct correlation with the latter, but only when a reverse shock is present. In this study, a similar exercise is repeated to establish how simulated peak intensities correlate with local compression ratios. Informed by the results from the previous section, it is assumed that the peak intensity occurs at the CIR trailing edge. Furthermore, given the emphasis on the number density in the previous section, the compression ratio of this quantity is considered along with that of the magnetic field for comparison with the results of *e.g.* Ebert *et al.* [2012]. This is repeated for observers E, B, and C, of Figure 6.7.

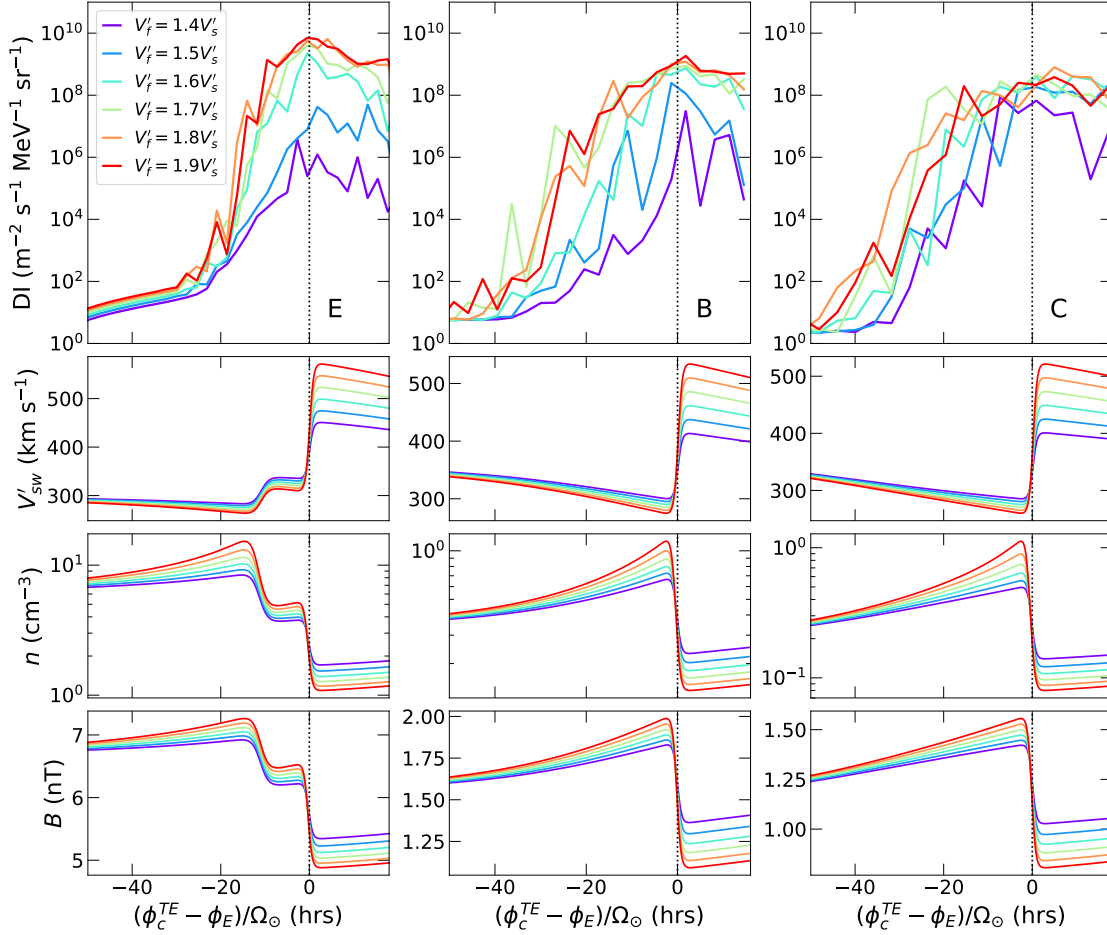


Figure 6.19: Similar to Figures 6.13 and 6.14, but only for the trailing edges (shown as vertical lines) and for varying values of V'_F as indicated in the legend. These profiles are shown for observers E, B, and C, as initially defined for Figure 6.7.

To simulate different compression ratios across the CIR trailing edge, the unperturbed fast SW speed V'_F is varied in Eq. 6.1. The value of the intermediate flow speed inside the interaction region is chosen purposefully to be low, that is, $V'_{SF} = 1.2V'_S$, to minimize the contribution of particles accelerated at the leading edge to intensities at the trailing edge. The resultant flow speed profiles, as viewed by each observer, along with the corresponding number density and magnetic field profiles are illustrated in Figure 6.19. Two flow speed values are identified to approximate the values up and downstream of the compression wave at the trailing edge, namely, the minimum flow speed between the SI and the trailing edge, and the maximum flow speed beyond the trailing edge. These values are used to calculate the corresponding values of the number density and magnetic field magnitude from Eqs. 4.14 and 5.16, respectively, from which, in turn, the compression ratios are calculated. These compression ratios are plotted in Figure 6.20 as functions of the ratios of the fast and slow SW speeds (V'_F/V'_S) considered for this section. The compression ratios scale proportional to V'_F/V'_S . However, for the same V'_F/V'_S -values, the factors by which the number densities and magnetic fields change across the trailing edge are larger for the observers that are further along the CIR.

The intensity profiles of 100 keV particles (assumed to have been accelerated at the trailing edge) are shown in the top panel of Figure 6.19. For larger V'_F/V'_S -values, and therefore larger compression ratios, the intensities at the trailing edge are generally higher. These profiles are

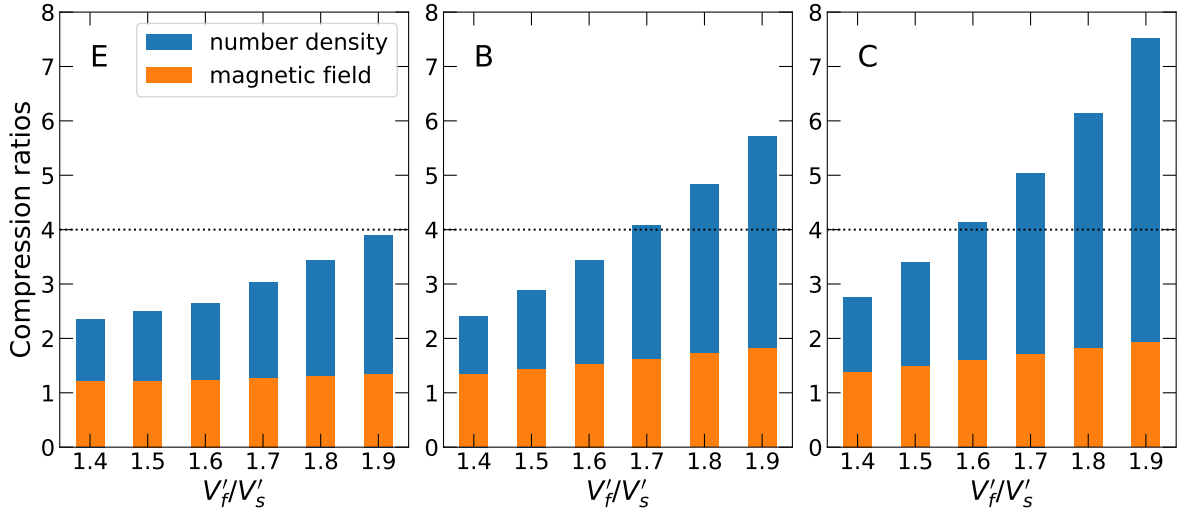


Figure 6.20: Number density and magnetic compression ratios as a function of the ratio between the fast and slow SW speeds. This is shown for the observers corresponding to each of the columns in Figure 6.19.

also broader for observers B and C at larger heliocentric distances. This is presumably because the diffusion coefficients are larger there, which allows particles to be transported further away from their source at the trailing edge. Note that the peak intensities at the trailing edge are very similar for the largest compression ratios (and quite generally for observer C in the rightmost panel). As encountered before in Figure 6.18, this follows because accelerated spectra adopt similar spectral indices near the maximum value of -1 when compression ratios are large (typically $\gtrsim 4$). It is shown in Figure 6.20 that there are only three and two cases of V_F'/V_S' -values, for observers B and C, respectively, for which the density compression ratio is smaller than 4. For all the other V_F'/V_S' -values, spectra would adopt a spectral index of approximately -1 . The spectral indices associated with the density compression ratios given in Figure 6.20 (calculated using 4.19) provide reasonably good fits for the power-law segments of the energy spectra corresponding to each V_F'/V_S' -value. This is illustrated for sample spectra in Figure 6.21. The variation of power-law indices gives rise to the trend of larger intensities following from larger compression ratios.

It remains to be quantified how well the simulated peak intensities scale with compression ratios. As an example, the peak intensities of 100 keV particles are plotted against their corresponding density and magnetic compression ratios in Figure 6.22. From the accompanying linear regression lines it can be inferred that the peak intensities of 100 keV particles and both sets of compression ratios are strongly correlated for observers E and B, with $R^2 \sim 0.9$. By contrast, the correlation is weak for observer C, as already inferred from the corresponding profiles in Figure 6.19. To obtain a complete perspective, this correlation test is repeated for several energies within the considered range from ~ 6 keV to 4 MeV. The results are collated by plotting R^2 as a function of energy in the top panel of Figure 6.23 for both sets of correlations. For observers E and B, for which spectra show meaningful variation in power-law indices with varying compression ratios, the linear regressions represent good fits at lower energies ($\lesssim 300$ keV). Note that the large depression in the R^2 -values centred about ~ 15 keV for observer E follows from the intersection of energy spectra around this point. This intersection is visible

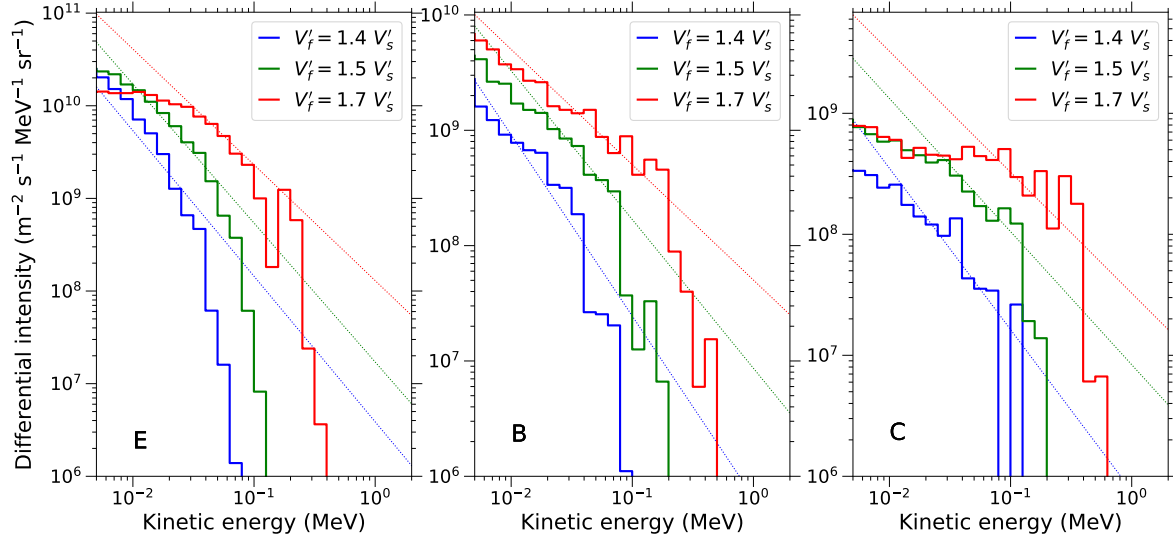


Figure 6.21: Sample energy spectra at the time of CIR trailing edge passages as viewed by the observers corresponding to each of the columns in Figure 6.19. The thin dotted lines represent fits to the power-law segments of spectra, with their spectral indices calculated using $(s + 2)/(2 - 2s)$ (Eq. 4.19) from the compression ratios for corresponding V_f'/V_s' -values in Figure 6.20.

in the leftmost panel of Figure 6.21 and is discussed further below. Note furthermore that at larger energies of the order of a few MeV, where accelerated spectra are in their exponentially decreasing phases, the correlations begin to diminish. Interestingly, at these large energies the correlations at observer C become comparable to those of the other observers, whereas the correlations at low energies are weak owing to spectra being similarly aligned with E^{-1} for different compression ratios. With their correlations being similar, the density and magnetic compression ratios appear to organize peak intensities comparably well.

The results of a statistical significance test (or ‘p-test’) are shown in the bottom panel of Figure 6.23, where the null hypothesis is that the slope of the relation between the peak intensities and compression ratios is zero. Disregarding the depression between ~ 8 and 25 keV arising from the intersection of spectra viewed by the observer at Earth, fair significance levels ($p \lesssim 0.01$) are implied for $E \lesssim 300$ keV and $E \lesssim 200$ keV for the relationships with the density and magnetic compression ratios, respectively. At these energies, the existence of a significant relationship is implied. As a possible result of the high levels of stochastic variation, significance levels are not consistently large at higher energies.

These results suggest that peak intensities scale with local compression ratios in an appreciably linear fashion on the conditions that energy spectra be power-law distributed (as would result from DSA) and that the density compression ratios are smaller than 4. Taken together with the fact that spectral indices of power-law distributed segments also relate to local compression ratios, this is indicative of local acceleration. However, the breakdown of the aforementioned relationship at the intersection of spectra as viewed by observer E (in the leftmost panel of Figure 6.21) suggest other processes are also involved.

This intersection of spectra follows as a result of the flattening of those associated with large compression ratios at lower energies. This is visible for observers E and C in Figure 6.21, as well as for spectra in Figure 6.18. Note that, in the context of processes included in the numerical

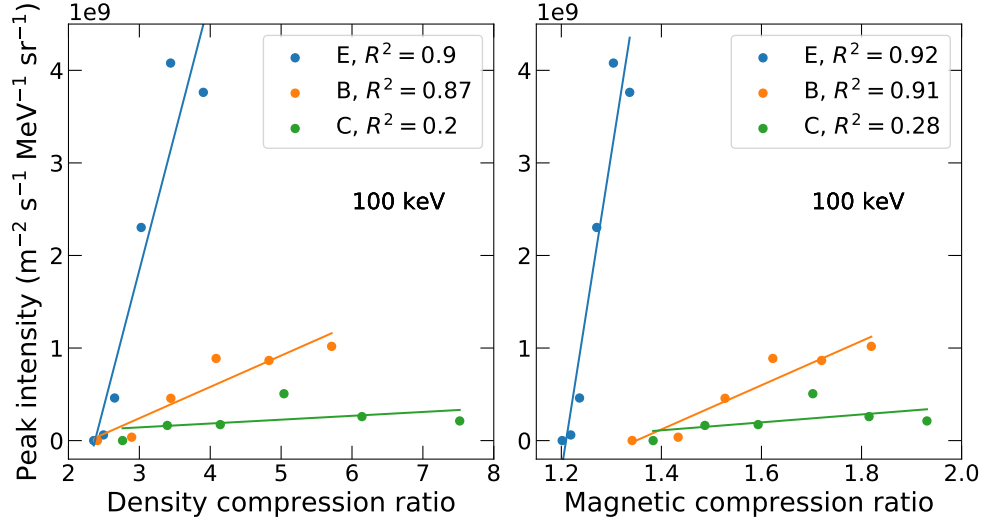


Figure 6.22: Sample scatter plots illustrating the relationship between peak intensities for 100 keV particles and local compression ratios at the CIR trailing edge for each of the observers in Figure 6.19. This is illustrated for compression ratios in the number density and magnetic field magnitudes as shown on the left and right, respectively. The R^2 -values in the legends indicate the goodness-of-fit for the linear regression lines in similar colors.

model, particles may be injected into the DSA process from the SW distribution during different stages of heating and at energies upward of a variable injection threshold. Indeed, Figures 6.5 and 6.6 illustrate large differences in the SW energy distribution directly before and after the trailing edge passage. The associated variation in the bulk and thermal speeds across this boundary further affects the injection efficiency [see also *Giacalone and Jokipii, 1997*], while Figure 6.19 demonstrates that these changes are more pronounced for larger compression ratios. The flattened spectra for large compression ratios, and their intersection with spectra associated with smaller compression ratios, then conceivably follow from a significantly heated SW distribution. In this case particles can be injected from the thermal core of the fast-stream SW distribution, which has been significantly shifted to higher energies with lower associated thermal peak intensities. This explains both why the intensities of these flattened spectra are lower at lower energies and why they extend to higher energies.

It is noted finally that, since the aforementioned explanation involves the transport of particles from adjacent flow regions to the trailing edge, the variable occurrence of the flattening effect (observed for observers A and C, but not for B) may be subject to favourable magnetic connections. However, this transport may also occur by means of perpendicular diffusion [*Dwyer et al., 1997*]. Low-energy particle intensities are disproportionately modulated during transport, which also has the effect of a low-energy downturn, especially if the source of the particles is remote [*Ebert et al., 2012; Yu et al., 2017*]. Indeed, complicated spectral forms may arise if locally accelerated spectra are contaminated by the modulated intensities of remotely accelerated particles. Non-local acceleration is explored further in Section 6.7.

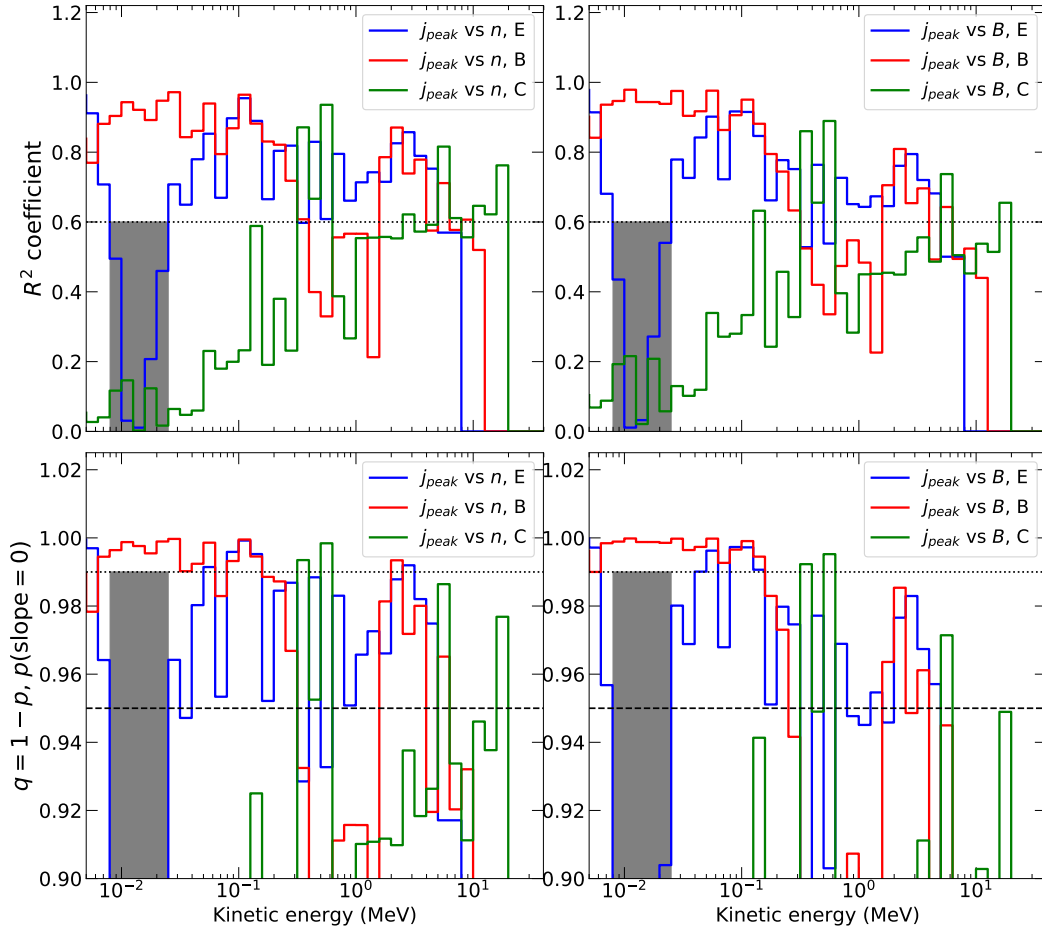


Figure 6.23: Top: R^2 coefficients measuring how well peak intensities correlate with local trailing edge compression ratios as a function of energy. This is shown for density and magnetic compression ratios, as shown on the left and right, respectively, and for the observers corresponding to each of those in Figure 6.21. The dotted horizontal line is an arbitrary guideline for the suitability of the linear fit. Bottom: Similar to the plots at the top, but for the $q(=1-p)$ -coefficient measuring the significance of the above correlations. Dashed and dotted horizontal lines respectively indicate the 95% and 99% confidence intervals that both quantities are linearly related. The shaded regions indicate the energies at which the correlation would appear small due to the intersection of spectra in the leftmost panel of Figure 6.21.

6.7 On the acceleration sites of CIR particles

The results from previous sections suggest that intensities generally peak near the CIR trailing edge, and that these peak intensities are related to local compression ratios (at least, up to a few hundred keV). These findings imply locally driven acceleration of CIR particles, presumably at a reverse compression wave or a shock associated with the trailing edge. However, this does not preclude particles accelerated elsewhere from being transported to the observer. To investigate this, the same technique applied in Section 4.6.3 is implemented, whereby pseudo particles are traced time-backwards from the observational point and their positions in terms of any pair of coordinates (r, ϕ, θ, E) binned at specified instances in time. Since pseudo particles are weighted according to particle amplitudes, how the particle amplitudes are distributed is indicative of the actual intensity contributions of particles transported from those locations. Using this method, the prior distributions of particles, in terms of (r, ϕ) and (r, E) , which would eventually contribute to 500 keV intensities at observers E and C at the moment of the trailing

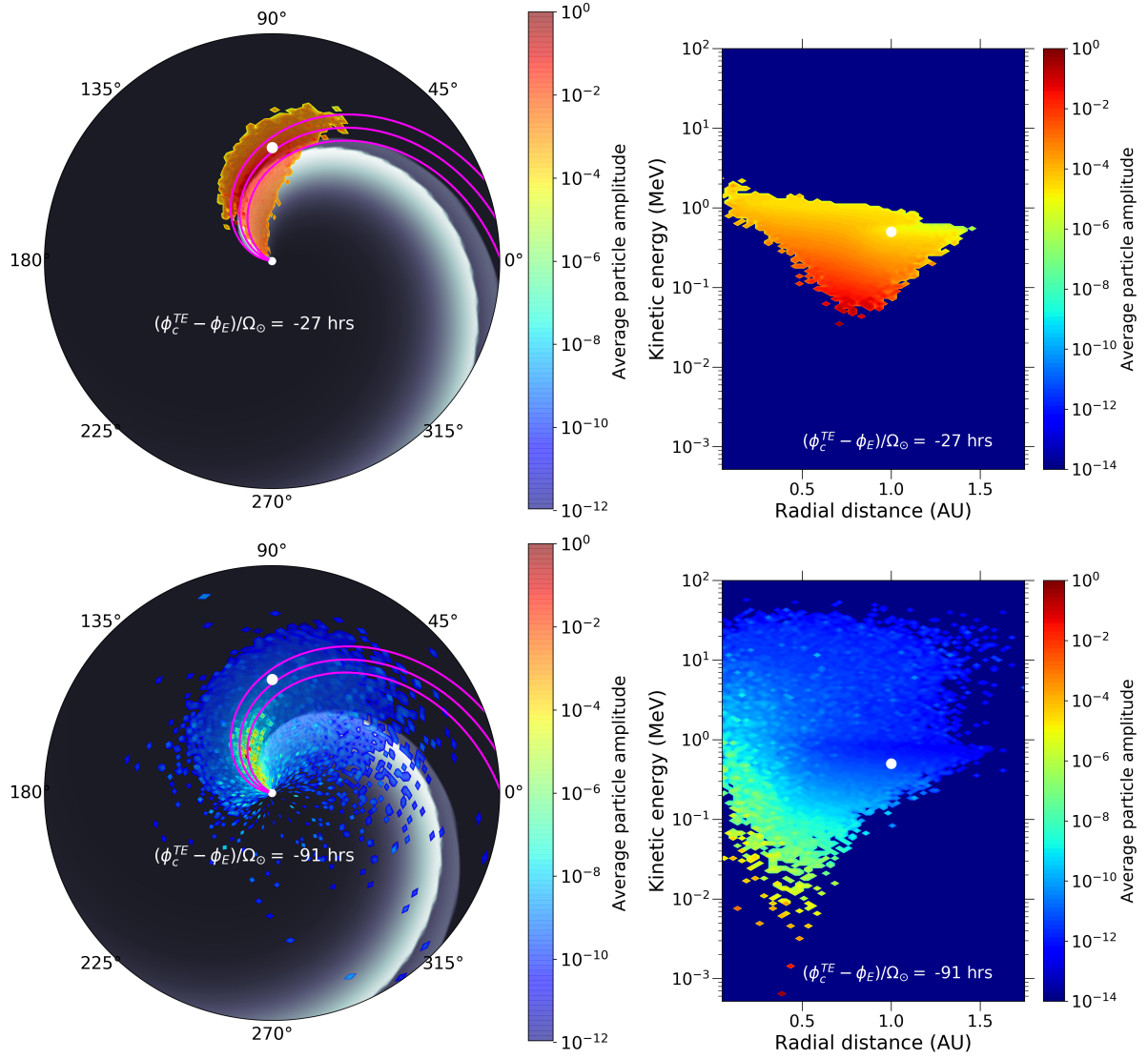


Figure 6.24: Prior distributions of CIR particles contributing to 500 keV intensities during the CIR trailing edge passage at Earth. Left: Similar to Figure 6.15, the color scale indicates normalized particle amplitudes at each point in the heliographic equatorial plane, shown for the indicated times prior to the trailing edge arrival. Right: Similar to Figure 4.18, with radial and energy distributions corresponding to the plots given for the same times on the left.

edge's arrival, are presented in Figures 6.24 and 6.25.

For the observer at Earth, in Figure 6.24, the distributions of contributing pseudo particles are respectively considered roughly one day and 4 days prior to the the arrival of the CIR trailing edge. Similar to Figure 6.15, flow speeds are included in the background of the spatial distribution plots so that the CIR's position can be tracked. Note that these plots are also normalized such that the maximum intensity contribution is unity. Therefore, at the moment of the trailing edge's arrival, the only populated part of the plot would be at the observer's location with a value of unity. The top left panel of Figure 6.24 shows that shortly before the arrival of the CIR, contributing particles are distributed fairly locally about the observational point and densely around field lines that are connected to the approaching CIR. This plot can be interpreted as revealing the acceleration site of the contributing particles at the approaching CIR, and that these particles are transported to the observer via a magnetic connection. Indeed, the bottom left

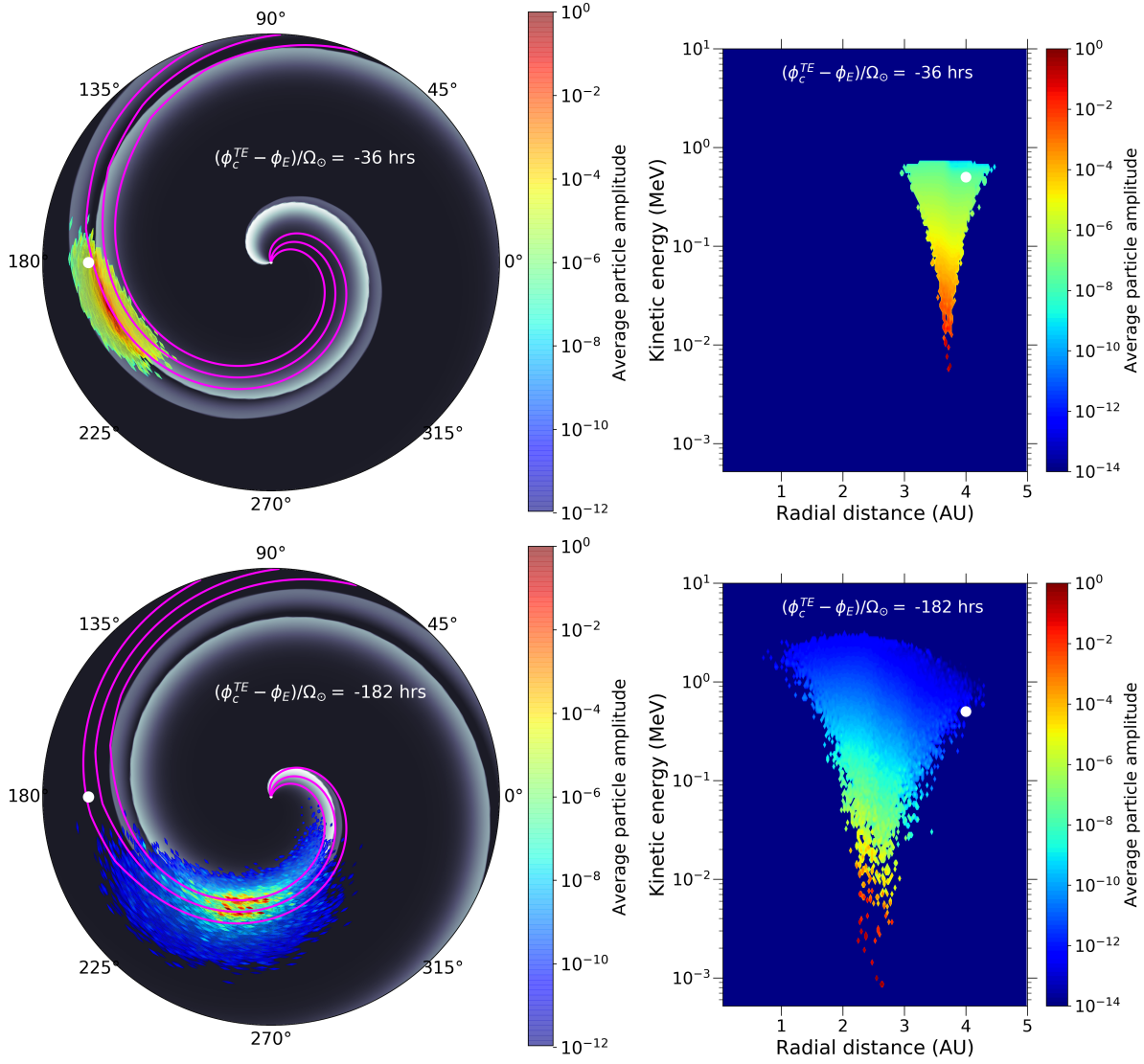


Figure 6.25: Similar to Figure 6.24, but shown for observer C as defined in Figure 6.1 at the coordinates $r_{\text{obs}} = 4$ AU and $\phi_{\text{obs}} = \phi_E = -180^\circ$.

panel similarly shows that at this earlier time the most significant contributions still emanate from particles magnetically connected to the observer from the even more distant CIR.

The adjacent plot, in the top right panel of Figure 6.24, shows that the largest contributions are from particles that at this time have energies of a few hundred keV and are stationed around ~ 0.75 AU. There is also a smaller contribution from MeV particles that would have to be decelerated through *e.g.* adiabatic energy losses to the target energy. Roughly another three days prior to this, the bottom right panel shows a seed population that is radially further removed from the observer, with significant contributions associated with particles at energies as low as ~ 1 keV. Considering Figure 6.12, injection thresholds in this region can be fairly low, and particles can therefore be injected upward of only a few keV. Note from the comparison of the top and bottom panels of Figure 6.24, the distributions shift to progressively higher energies and larger radial distances with time as the CIR progresses toward the observer, indicative of continual acceleration at the CIR.

Figure 6.25 depicts a similar situation for observer C at a heliocentric distance of 4 AU. In the

top panel, at a time where the observer is already within the interaction region, but preceding the arrival of the trailing edge, contributing particles are once again distributed closely along field lines. In this case they are magnetically connected with the approaching reverse compression wave at the trailing edge. The largest intensity contributions emanate from an extended region along the trailing edge: this contributing population is radially removed from the observer by less than 0.5 AU, but extends nearly 40° azimuthally. This follows because field lines run along the compression wave front for some distance. Over a week prior to this, as shown in the bottom left panel of Figure 6.25, the most significantly contributing particles are similarly distributed along field lines running along both the leading and trailing edges of the CIR, with a better magnetic connection to the observer from the former. Note that it is possible for particles to be transported from the trailing edge to better connected field lines by means of cross-field diffusion. In this case, the largest contributions are associated with particles that are between 1 and 2 AU removed from the observer and separated by up to $\sim 90^\circ$ azimuthally.

In terms of energy, the adjacent plots in Figure 6.25 show that over a day prior to the arrival of the trailing edge, the most significant contributions are associated with $\sim 10\text{--}100$ keV particles. Injection energy thresholds in the area around observer C are expected from Figure 6.12 to be higher than nearer to Earth, and the more locally accelerated particles would have had to be accelerated to sufficiently high energies prior to the arrival of the CIR. Indeed, the bottom right plot of Figure 6.25, which corresponds to when the CIR was at smaller heliocentric distances in regions with lower injection thresholds, shows particles accelerated from energies as low as a few keV. In this manner, non-local prior acceleration can make meaningful contributions to the intensity enhancements observed later at the time of the trailing edge's passage. In any event, remote acceleration sites most often correspond to magnetically connected regions along the CIR trailing edge.

The non-local acceleration referenced here should not be confused with the sunward streaming of CIR particles accelerated at a few AU [Richardson *et al.*, 1993; Scholer *et al.*, 1999]. The transport of particles in this study is considered in the diffusive limit, with movement along field lines governed by parallel diffusion, which is a comparatively slow process. Streaming particles also have large MFPs, which contrasts with the strong scattering assumed in this study. It is within this strong scattering limit that DSA can be considered an effective acceleration mechanism.

6.8 Summary and conclusions

In this chapter, SDEs equivalent to the 3D Parker [1965a] TPE are solved to simulate the acceleration of particles at compression regions associated with CIRs. The SW properties associated with the CIR are described using an analytical model, and the source function is specified similarly to previous chapters in terms of a preheated suprathermal SW distribution. Moreover, a variable injection energy threshold is implemented that is based on the relative obliquity of CIR-associated compression waves and local magnetic fields. A modification to the standard Parker [1958] spiral is furthermore implemented to ensure a divergence-free magnetic field in compression regions. Despite appreciable θ -components following from this modification, the intensities of accelerated particles viewed by observers based in the heliographic equatorial

plane are negligibly affected. It is therefore shown that solving the SDEs for only two spatial coordinates (namely, r and ϕ) yields serviceable approximations for 3D TPE solutions, given that particle transport is reasonably limited to the equatorial plane.

Applying the aforementioned model for a typical CIR SW configuration [e.g. *Belcher and Davis, 1971*], the salient features of intensity-time profiles observed during the passage of CIRs are reproduced: a sharp onset of particle enhancements is followed by a peak in intensities at or near the trailing edge of the interaction region, followed by a more gradual decrease of intensities in the rarefaction region. The simulated intensities of $\sim 0.1 - 0.5$ MeV CIR particles consistently peak near the trailing edge, even in the event that compression ratios at the leading edge are comparable. It is argued that this may follow owing to a combination of factors. Firstly, intensities may peak at the trailing edge because of the accumulation of particles accelerated prior to its arrival, either at the leading edge or between converging scattering centres inside the interaction region [e.g. *Giacone et al., 2002*]. Secondly, it may follow because of local transport conditions. In the frame corotating with the Sun, randomly diffusing particles inside the interaction region are transported toward the trailing edge, while enhanced flow speeds beyond this boundary act in the opposite direction. Smaller diffusion length scales in the fast stream impede particles' escape across the trailing edge. Collectively, these factors create favourable conditions for acceleration at the trailing edge.

The intensities at either edge also increase proportional to larger local compression ratios. It is illustrated that this follows because spectral indices in the immediate vicinity of compression waves scale according to the local density compression ratios in a manner that is consistent with the predictions of DSA. The larger spectral indices that result from larger compression ratios raise intensities, especially at the higher-energy end of power-law distributed spectra. This indicates a causal relationship between peak intensities and local density compression ratios. Indeed, having analyzed their correlations across a broad range of energies, it is found that peak intensities scale with local compression ratios in an appreciably linear fashion up to ~ 300 keV. More generally, this proportionality can be considered valid within the energy range where spectra are power-law distributed, and for compression ratios that are small enough (typically, $s < 4$) for these power-law indices to respond to their variation. As a proxy for the same effect, magnetic compression ratios fare comparably well in organizing peak intensities [*Ebert et al., 2012*].

The dependence of peak intensities on local compression ratios is suggestive of locally driven acceleration. *Local acceleration* in this context refers to acceleration taking place at the observer during the passage of the compression wave. However, whereas the predominant contribution to peak intensities may indeed be attributed to particles accelerated in its immediate vicinity, it is shown that meaningful contributions to this intensity may be associated with particles accelerated elsewhere. Tracing pseudo particles weighted according to their particle amplitudes back to prior positions, it is revealed that remote acceleration sites are typically regions along the approaching CIR (and particularly its trailing edge) that are magnetically connected to the observer. Recall that since particle transport is considered in the diffusive limit, field-aligned transport occurs by means of parallel diffusion. In addition to the contributions made to intensities by these non-locally accelerated particles, it is also shown that prior acceleration at these

remote sites may be necessary to energize particles enough to overcome injection thresholds for local acceleration.

Interestingly, the aforementioned results are similar to those of *Zhao et al.* [2016], where the focused TPE was solved to reproduce CIR particle events observed in February 2008. While Section 5.5 draws a number of distinctions between diffusive and streaming-limited transport, the focused and *Parker* [1965a] TPEs may produce comparable results for strong magnetic turbulence. Notwithstanding those differences, *Zhao et al.* [2016] report that energetic particle spectra corresponding to the *in situ* measurement of a CIR reverse shock resemble those of the locally accelerated power-law spectra found in this study. Moreover, in the case considered by *Zhao et al.* [2016] where the observer is an appreciable distance removed, but magnetically connected to the shock, spectra show similarly large levels of modulation at sub-MeV/nucleon energies as evinced by low-energy downturns in otherwise power-law distributed spectra. That study does not explicitly consider particle acceleration at shocks and also neglects cross-field diffusion, which the authors argue would decrease the severity of modulation effects if included. Since the transport model in the present study includes those effects, but cannot account for transport in the streaming limit, the development of a model that combines these processes to study CIR particle acceleration and transport is an intriguing avenue for future work.

It is noted finally that the SDE solutions tend to show large statistical fluctuations in simulated differential intensities. This is in part owing to the complexity of the model, which includes *e.g.* variable injection energies and extended source regions with variable magnetic connections to observers. Although these fluctuations can be decreased by executing the model for larger numbers of pseudo particles, this is subject to the availability of computational resources. However, should more pseudo particles be employed, solutions are expected to remain qualitatively unchanged, albeit with less statistical variation.

Chapter 7

Discussion and conclusions

This study investigates the acceleration of energetic particles at shocks in the inner heliosphere. More specifically, the acceleration and transport of these particles observed during ESP events, coinciding with the passages of CME-driven shocks or associated with CIRs, is explored. This investigation is conducted by numerically modelling the major physical processes governing the acceleration and transport of the particles during the aforementioned events, including, in particular, the process of DSA. This study considers the thermal and suprathermal components of the SW particle distribution as a source from which these energetic particles may be accelerated. The acceleration of these SW particles at shocks, or generally, within regions of compressed SW flow, as well as their subsequent transport are simulated by means of the *Parker* [1965a] TPE. This TPE is solved for a near-isotropic particle distribution, and therefore particle transport is considered in the diffusive limit. This approach is applicable to the simulation of particle events associated with small anisotropies and strong scattering conditions, which are also typical requirements for effective DSA. Full descriptions of the underlying physical assumptions and the transport configuration used in this study are provided in **Chapters 2 and 3**.

Furthermore, **Chapter 3** discusses the solution of the TPE, which in this study is performed by means of the time-backward integration of an equivalent set of SDEs. Even though this approach limits applications to the test-particle case, it is advantageous in several ways. The independence of the simulated pseudo particle trajectories makes the SDE approach suitable for implementation on parallel computing platforms, while its numerical stability allows for the handling of large flow speed gradients (such as at shocks) and multiple computational dimensions (*e.g.* three spatial dimensions and energy). The values of distribution functions are conserved along the trajectories obtained when solving the SDEs for each coordinate. The average of the distribution function values, calculated at the coordinate values occupied by pseudo particles when the simulation time has elapsed, therefore gives the value of the distribution function at the observational point. When modelling DSA, the distribution function is only assigned a value if a trajectory intersects the shock, whereas changes in coordinate values are governed by the processes contained in the TPE. Using this SDE approach, the conditions and mechanisms required for simulating DSA are implicitly accounted for.

The outcomes of the study are discussed here according to the broad scientific themes set out

in **Chapter 1**, and not necessarily in the order that each of the research chapters is presented.

The classical features of DSA are visible in a number of instances throughout the study. The penultimate section of **Chapter 3** introduces these features, while **Chapter 4** discusses them formally. Most notably, power-law distributed energy spectra at shocks, or where shocks pass observers, are ubiquitous in the simulations. As expected from DSA, these power laws are arranged according to spectral indices that depend on the shock compression ratio, but only if the required length-scale hierarchy is observed [see *e.g.* Jones and Ellison, 1991]. If, for instance, particles' diffusion length scales are smaller than the thickness of the shock, the sampled compression ratio will only be a fraction of the total, which is reflected in energy spectra by softer power-law distributions. It is also shown that these shock accelerated power-law distributions only extend up to such energies as can be attained in the available acceleration time [Drury, 1983]. Above these energies, intensities of shock-accelerated particles decrease exponentially. The aforementioned DSA properties are encountered for each of the applications considered in the present study.

The comparative acceleration efficiencies of fast and strong shocks are evaluated in **Chapter 4** for simulated ESP events. Fast shocks are shown to produce a larger number of high-energy particles, owing to larger energy gains per shock crossing, allowing spectra to extend to higher energies within the available time. For strong shocks, with large compression ratios, spectra are harder, increasing the overall fluences of shock-accelerated particles. Both fast and strong shocks are therefore conducive to efficient acceleration [Lario *et al.*, 2005b; Mäkelä *et al.*, 2011; Giacalone, 2012]. However, simulations suggest that slow-moving strong shocks produce a greater number of energetic particles than fast-moving weak shocks.

Moreover, it is shown in **Chapter 6** that, for CIR particles whose intensities tend to peak at roughly the same time as the passage of the CIR's trailing edge [*e.g.* Desai *et al.*, 1998; Ebert *et al.*, 2012], the peak intensities scale proportionally to local compression ratios, but only at energies where spectra conform to the DSA-predicted power-law form. This may follow because of the relationship that exists between compression ratios and the power-law indices of shock-accelerated energy distributions. Harder spectra associated with large compression ratios yield higher intensities overall. However, the variation of spectral indices becomes less pronounced in the limit where compression ratios tend toward strong shock values of ~ 4 . This may explain why the correlation between the peak intensities and local compression ratios breaks down when densities vary by larger factors across the compression region.

The appearance of these DSA-associated spectral features may also be considered to be indicative of local acceleration, since these features are typically seen upon the arrival of a shock at the observer. During ESP events, as simulated in the penultimate section of **Chapter 4**, the spectrum at the time of the shock's arrival resembles the typical power-law form expected of shock-accelerated energy distributions, whereas during the shock's approach spectra show significant downturns at lower energies. These downturns are the consequence of low-energy particles being disproportionately modulated during their transport from the shock to the observer, which, in the context of the processes included in the numerical model, results from either rigidity-dependent diffusion or adiabatic cooling. Simulations furthermore show that this modulation of remotely accelerated spectra reproduces the observed spectral flattening of

suprathermal protons observed [by *e.g.* Lario *et al.*, 2018] ahead of the shock's arrival.

Similar results are presented in **Chapter 5** for shocks of finite longitudinal extent. The intensity profiles and energy spectra simulated for an observer in the direct path of the shock resemble those observed for typical ESP events. However, the energy spectra viewed by an observer that is not in the direct path of the shock, but is instead magnetically connected to the shock, resemble modulated forms of the typical shock-accelerated spectrum and show appreciable downturns at lower energies. For these observers, the DSA-associated power law does not extend down to the injection energy, because none of the particles contributing to intensities here are accelerated locally. Instead, they are accelerated remotely and modulated during their transport to the observer along magnetic field lines. In the diffusive limit, particles move along field lines by means of parallel diffusion. Whereas parallel diffusion is much more efficient than cross-field diffusion, the latter process modulates intensities appreciably when large enough to transport particles away from field lines connecting the shock and the observer.

Magnetic connections are revealed to be a major organizing factor in the transport of particles from remote acceleration sites. Whereas an observer in the shock's direct path usually sees accelerated particle intensities peak at the moment of the shock's arrival, for an observer outside of the shock's path intensities do not necessarily peak at the moment of the shock's closest approach. Instead, depending on the field-line geometry, intensities may peak either before or after the shock's closest approach, owing respectively to whether favourable magnetic connections could be established during the shock's approach or during its continued movement beyond the observer. This is reminiscent of the description of longitudinally dependent SEP transport by Reames [1999], but with the notable distinction that the present study considers transport in the diffusive limit, and only of particles accelerated from the SW.

This field-aligned transport is also demonstrated using a technique that is applied repeatedly in **Chapters 4** to **6**. The technique, utilizing a feature unique to the SDE approach, entails the construction of distributions of pseudo particles that are traced backwards in time from observational points and weighted according to their interactions with the shock. This reveals the probable spatial and energy distributions of particles that would eventually contribute to intensities at a particular energy as viewed by an observer at a particular point in space and time. As illustrated in *e.g.* **Chapter 5**, these prior distributions show that a fraction of the particles contributing to intensities during ESP events is indeed accelerated remotely, and perhaps continually for particles keeping pace with the shock. The concentration of these particle distributions along magnetic field lines demonstrate the importance of magnetic connections for transport between the shock and the observer.

Applying the same technique to construct the prior distributions of particles contributing to intensities during a CIR event, a fraction of the particles is similarly shown in **Chapter 6** to be transported from remote acceleration sites. These sites include, but are not limited to, points along the trailing edge of the approaching CIR. Given that injection energy thresholds may vary as a result of the relative geometries of magnetic field lines and the compression waves bounding the CIR, prior acceleration at remote sites may be necessary to adequately energize particles to overcome injection thresholds for local acceleration. Indeed, simulated energy spectra at CIR trailing edges reflect mixed signatures of local and remote acceleration, often display-

ing the DSA-predicted power law at high energies, but with extended flattening suggestive of modulation at low energies. This conceivably follows because of the accumulation of particles at the trailing edge that were accelerated either locally (at the trailing edge itself), between converging scattering centres within the adjacent interaction region [Jokipii *et al.*, 2001; Giacalone *et al.*, 2002], or at remote sites along the CIR. It may therefore be reasonable to expect that DSA signatures may often be concealed in observations of CIR particles. However, the contributions of at least those particles accelerated on the leading edge's side of the CIR may be neglected, because such particles would have difficulty crossing the stream interface considering that in reality, field lines in the slow and fast SW streams do not interpenetrate.

A distinctive feature of the present study is the transformation of the SW distribution during the passage of shocks or compression waves. This is introduced and discussed in **Chapter 4**, and essentially transforms the source function from which particles are accelerated. Considering the intricate arrangement of flow regions inside CIRs, and that the SW velocity divergence within these regions is typically nonzero throughout, it is apparent that particles will be accelerated from the SW distribution in various stages of its evolution. This further contributes to the complexity of CIR particle spectra simulated in **Chapter 6**. Nevertheless, given the ubiquity of suprathermal tails in the SW, and similar compositions [Mason *et al.*, 2008, 2012; Bučík *et al.*, 2012], the suprathermal SW distribution serves as a likely candidate for an extended source for DSA in CIRs [see also Filwett *et al.*, 2017; Yu *et al.*, 2017]. Moreover, as shown in the penultimate section of **Chapter 4**, the prior heating of the SW distribution may be necessary to reproduce the intensities of typical ESP events, especially if injection energy thresholds are high [see also Prinsloo *et al.*, 2019]. Similar reasoning may apply for shock waves associated with CIRs.

This study, and the models developed herein, may be expanded or adapted in a number of ways to pursue further avenues of research. These include:

- Expanding the study to investigate the acceleration of other species of energetic particles.
- Including improved turbulence-based descriptions of diffusion coefficients.
- Modelling the effects of drifts in the TPE. This would require the inclusion of a 3D heliospheric current sheet in the SDE model [see *e.g.* Engelbrecht *et al.*, 2019, and the references therein]. This may be useful to study the effects of current sheets on CIR particle transport and acceleration.
- Coupling the SDE model with MHD models for more realistic representations of the SW and magnetic fields, especially with respect to the descriptions of CMEs [*e.g.* Hu *et al.*, 2017; Scolini *et al.*, 2019] and CIRs [*e.g.* Wiengarten *et al.*, 2014; Wijsen *et al.*, 2019].
- Constructing a similar SDE model based on focused transport equations [le Roux and Webb, 2012] to simulate particle events with large anisotropies.
- Including similar descriptions of *e.g.* the evolution of the SW distribution in transport models capable of simulating non-linear effects, such as particle-mediated shock modification [Mostafavi *et al.*, 2017] or self-generated turbulence by means of wave generation [Lee, 1983; le Roux and Arthur, 2017].

Appendices

Appendix A

On the normalization of the kappa function

The normalization constant A_κ of the standard κ -function introduced in Eq. 2.5 is obtained by setting its integral over all phase space equal to the number density of the solar wind. Assuming an omni-directional (or three-dimensional) κ -function, averaged as per Eq. 3.4, the expression given in Eq. 3.5 can be used to calculate the normalization constant. Note, however, because f_κ is often expressed as a function of velocity instead of momentum, the analogous expression in velocity coordinates, namely

$$n_{sw} = \int_0^\infty 4\pi v^2 f_\kappa(v) dv, \quad (\text{A.1})$$

is used to calculate the number density, denoted here as n_{sw} , and not n , as used in the main text, to differentiate from the n^{th} -order moments referenced below. Bear in mind that for use in the transport equation, e.g. when specifying f_s in the source function, the conversion $f_s = f_\kappa/m_p^3$ applies, because $\int 4\pi p^2 f_s dp = \int 4\pi (m_p v)^2 f_s d(m_p v) \equiv \int 4\pi v^2 f_\kappa dv$. Here, only the proton rest mass m_p is used, since this study is concerned with solar wind protons with kinetic energies typically much smaller than their rest-mass energy. A non-relativistic description is therefore applicable. Note furthermore that Eq. A.1 is also known as the zeroth-order velocity moment of f_κ , and that it can be cast into a more general form for the n^{th} -order moment, namely

$$\langle v^n \rangle = \int_0^\infty 4\pi v^{n+2} f_\kappa(v) dv, \quad (\text{A.2})$$

which, upon substituting Eq. 2.5, becomes

$$\langle v^n \rangle = 4\pi A_\kappa \int_0^\infty v^{n+2} \left(1 + \frac{v^2}{\kappa v_\kappa^2}\right)^{-(\kappa+1)} dv, \quad (\text{A.3})$$

from which the normalization constant A_κ can be calculated. The integral in Eq. A.3 is evaluated by applying the transformation $v^2/(\kappa v_\kappa^2) \rightarrow \eta$, which allows the expression to be rewritten

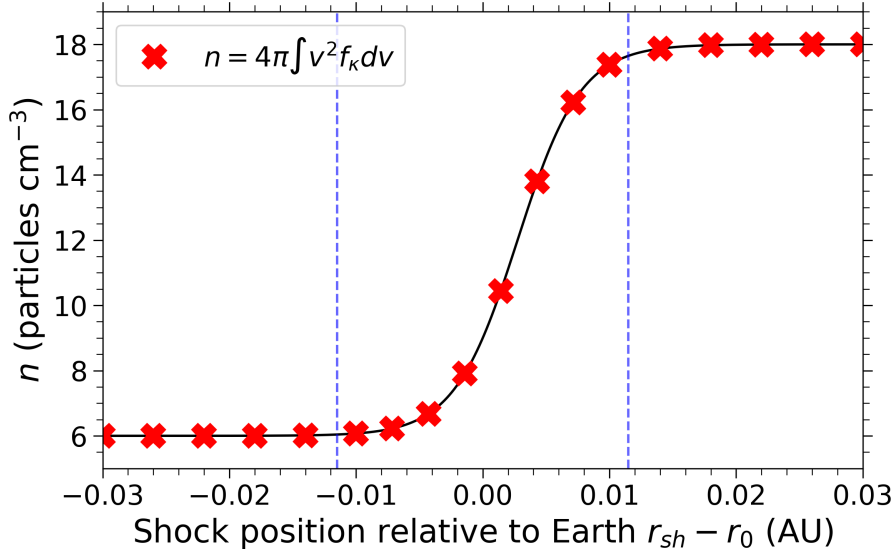


Figure A.1: SW number density profile corresponding to the same profile shown in Figure 4.2. The red markers are the values of the integral in Eq. A.1 for different stages during the shock passage. Similar to Fig. 4.2, the vertical lines indicate the extent of the shock region.

as

$$\langle v^n \rangle = 2\pi A_\kappa (\kappa v_\kappa^2)^{(n+3)/2} \int_0^\infty \eta^{(n+1)/2} (1+\eta)^{-(\kappa+1)} d\eta. \quad (\text{A.4})$$

Note that the integral is now in the form of the β -function, given by

$$\beta(x, y) = \int_0^\infty \eta^{x-1} (1+\eta)^{-(x+y)} d\eta = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}. \quad (\text{A.5})$$

Recognizing that $x = (n+3)/2$, $y = \kappa - (n+1)/2$, and $x+y = \kappa+1$, the integral in Eq. A.4 can be solved by invoking the identity given in Eq. A.5, so that

$$\langle v^n \rangle = 2\pi A_\kappa (\kappa v_\kappa^2)^{(n+3)/2} \frac{\Gamma((n+3)/2)\Gamma(\kappa - (n+1)/2)}{\Gamma(\kappa+1)}, \quad (\text{A.6})$$

from which the normalization constant can be determined as

$$A_\kappa = \frac{n_{sw}}{2\pi(\kappa v_\kappa^2)^{3/2}} \frac{\Gamma(\kappa+1)}{\Gamma(3/2)\Gamma(\kappa-1/2)} \quad (\text{A.7})$$

by setting $\langle v^{n=0} \rangle = n_{sw}$, yielding the same expression given in Eq. 2.7. The standard kappa function is hence given by

$$f_\kappa = \frac{n_{sw}}{2\pi(\kappa v_\kappa^2)^{3/2}} \frac{\Gamma(\kappa+1)}{\Gamma(3/2)\Gamma(\kappa-1/2)} \left(1 + \frac{v^2}{\kappa v_\kappa^2}\right)^{-\kappa-1}. \quad (\text{A.8})$$

Figure A.1 illustrates the normalization of the κ -function, showing that the values of the integral in Eq. A.1 does indeed trace the SW number density, as intended.

Appendix B

Supplemental content on stochastic differential equations

B.1 Equivalence of SDE and finite-difference numerical methods: Application to an event during the 2003 Halloween epoch

In a similar study, where DSA is also assumed as an acceleration mechanism when simulating ESP events, *Giacone* [2015] utilizes a finite-difference numerical scheme to solve the *Parker* [1965a] TPE in a single spatial dimension for a strong fast-moving shock ($V_{sh} = 1900 \text{ km s}^{-1}$, $s = 4$). In that study, the energetic particle event, or *Halloween* event, of 2003 October 29 is considered as an application for which observed energy spectra and temporal profiles are reproduced. To demonstrate their equivalence as numerical methods, the SDE approach of this study is implemented to reproduce particle intensities for the same event using a similar parameter configuration to that of *Giacone* [2015]. The source function in that study is bound to a numerical grid, which does not exist in the SDE approach. For the purposes of this application, the source function is instead specified directly at the shock as a very soft power law in momentum (p^{-7}), where simulated intensities are retroactively normalised to observed intensities. Furthermore, the diffusion coefficient is implemented as specified by *Giacone* [2015], that is, of order $10^{19} \text{ cm}^2 \text{ s}^{-1}$ near the Sun and with a momentum dependence of $\sim p^{1.5}$.

The resultant energy spectra and time profiles of energetic particle intensities are shown in Figure B.1. Overall, the finite-difference and SDE solutions are similar. Recall that the SDEs must be solved for a large number of pseudo particles for each energy, position or point in time at which intensities are sought. The resolution of SDE solutions therefore merely depends on the number of times the simulation is repeated and how the observational points are distributed, as opposed to the fixed grid resolution of finite-difference schemes. For example, in Figure B.1, a larger number of observational points are chosen in energy than in time, as shown in the left and right-hand side panels, respectively. Note that the SDE solutions tend to slightly undershoot the finite-difference solutions where steeper gradients exist. This presumably follows because there is no passage of information between pseudo particles and their associated observational points as would exist between adjacent points in finite-difference schemes. The SDEs typically yield less gradual intensity gradients as a result. This is useful to bear in mind when

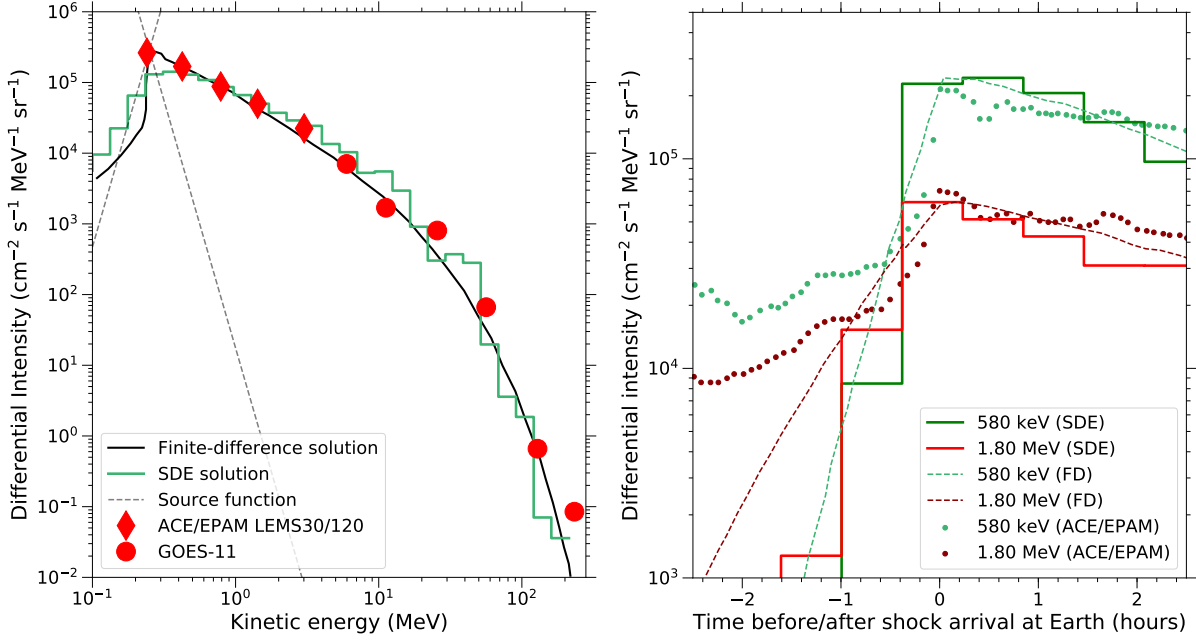


Figure B.1: Left: Energy spectra at Earth's position at the time of a CME-driven shock passage on 2003 October 29. Using similar parameter configurations, solutions of the SDE approach used in this study and the finite-difference method of *Giagalone* [2015] are shown in solid green step-like and black lines, respectively. The red diamond and circle markers represent observations from ACE/EPAM (LEMS30 and LEMS120) and GOES-11, respectively. Right: Temporal profiles of 580 keV and 1.8 MeV ion intensities as observed at Earth during the same event considered on the left. The SDE and finite-difference solutions are shown as solid step-like and dashed lines, respectively, while dot-markers indicate observations from ACE/EPAM (LEMS30 and LEMS120). See *Giagalone* [2015] and the references therein for details.

fitting functions to shock-accelerated spectra simulated using these two approaches, since the high-energy cut-off is likely to be more abrupt for the SDEs than for finite-difference solutions.

Note, as an aside, that simulated intensities of either method reproduce observations better near the shock than away from it. This follows since the only source of particles in the simulations is situated on the shock itself, while the observed intensities include contributions from other sources, leading to a high background intensity. The comparison of the simulations generated using the two different numerical methods demonstrate the equivalence of their results, and therefore also demonstrates the validity of the numerical approach implemented in this study.

B.2 Time-forward transport equation with importance sampling

To infer the SDEs for time-forward integration, Eq. 3.42 must be rewritten in conservative form, resembling the time-forward Kolmogorov equation of Eq. 3.35. This entails many steps of arithmetic, although only a contracted outline is provided here.

Applying the product rule of differentiation in reverse to each term in Eq. 3.42, with $1/A$ factored out, one obtains

$$\frac{\partial h}{\partial t'} = \frac{1}{A} \left(-\frac{\partial}{\partial x} \left(\left(\frac{\partial \kappa}{\partial x} + V \right) Ah \right) + \frac{\partial^2}{\partial x^2} (\kappa Ah) + \frac{1}{3} \frac{dV}{dx} \frac{\partial}{\partial p} (pAh) + \frac{2}{3} \frac{dV}{dx} Ah \right), \quad (\text{B.1})$$

which, when multiplied throughout with p^2 , and noting that

$$\frac{\partial}{\partial p} (p^2 \cdot ph) = p^2 \left(\frac{\partial}{\partial p} (ph) + 2h \right), \quad (\text{B.2})$$

becomes

$$p^2 \frac{\partial h}{\partial t'} = \frac{1}{A} \left(-\frac{\partial}{\partial x} \left(\left(\frac{\partial \kappa}{\partial x} + V \right) p^2 Ah \right) + \frac{\partial^2}{\partial x^2} (\kappa p^2 Ah) + \frac{1}{3} \frac{dV}{dx} \frac{\partial}{\partial p} (p^2 \cdot pAh) \right). \quad (\text{B.3})$$

Applying the transformation $H = p^2 h$, this can be rewritten as

$$\frac{\partial H}{\partial t'} = -\frac{1}{A} \frac{\partial}{\partial x} \left(\left(\frac{\partial \kappa}{\partial x} + V \right) AH \right) + \frac{1}{A} \frac{\partial^2}{\partial x^2} (\kappa AH) + \frac{1}{3} \frac{dV}{dx} \frac{\partial}{\partial p} (pH). \quad (\text{B.4})$$

Recall that $A = A(x)$ is not a function of p . Finally, terms that contain the $1/A$ factor are rewritten in conservation-law form, again by applying the product rule in reverse, to yield

$$\frac{\partial H}{\partial t'} = -\frac{\partial}{\partial x} (a_x H) + \frac{1}{2} \frac{\partial^2}{\partial x^2} (c_{xx} H) - \frac{\partial}{\partial p} (a_p H) + \mathcal{L}H, \quad (\text{B.5})$$

which is in the form of the time-forward Kolmogorov equation (Eq. 3.35). The coefficients are given by

$$a_x = \frac{\partial \kappa}{\partial x} + V - \frac{2\kappa}{A} \frac{dA}{dx}, \quad (\text{B.6})$$

$$a_p = -\frac{p}{3} \frac{dV}{dx}, \quad (\text{B.7})$$

$$c_{xx} = 2\kappa, \quad (\text{B.8})$$

and

$$\mathcal{L} = -\left(\frac{\partial \kappa}{\partial x} + V - \frac{2\kappa}{A} \frac{dA}{dx} \right) \frac{1}{A} \frac{dA}{dx} - \frac{\kappa}{A} \frac{d^2 A}{dx^2}. \quad (\text{B.9})$$

In the main text, the TPE is given in the form of Eq. B.5 in Eq. 3.36, from which the equivalent time-forward SDEs may be inferred.

Appendix C

Transformation of flow speeds between the spacecraft and shock frame

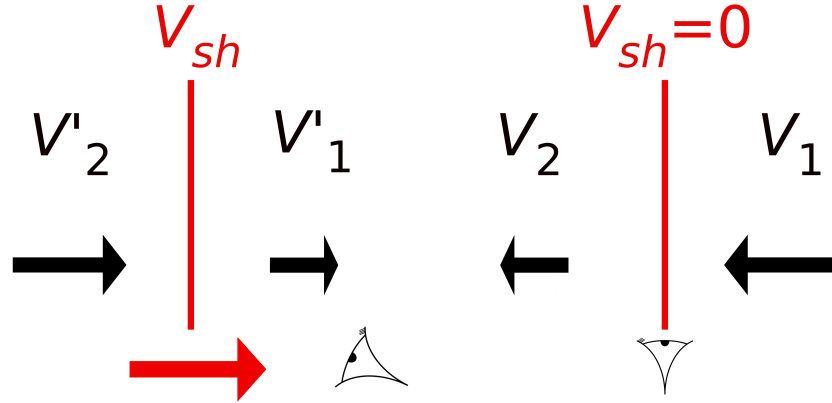


Figure C.1: Flow speeds as viewed by an observer in the spacecraft frame (as shown on the left) and an observer moving with the shock (as shown on the right). The symbols V_1 and V_2 are the upstream and downstream flow speeds in the rest frame of the shock. The corresponding primed symbols are the flow speeds in the spacecraft frame. The shock speed in each frame is represented by V_{sh} . Arrows indicate the directions of flow and their lengths represent the relative magnitudes of the flow speeds.

Consider a spherical CME-driven interplanetary shock with speed V_{sh} in both the spacecraft and shock frames as illustrated in Figure C.1. Note that the numbers 1 and 2 denote upstream and downstream flow speeds, respectively, whereas primed and unprimed flow speeds represent SW speeds in the spacecraft (or fixed) frame and the shock frame, respectively. Suppose the undisturbed upstream SW flow speed as observed by a spacecraft is V'_1 . In the rest-frame of the shock (for an observer travelling at the same speed as the shock), the shock appears stationary. Transforming speeds to the shock frame requires the shock speed V_{sh} to be subtracted throughout, including from itself. The upstream shock-frame flow speed V_1 is therefore given in terms of non-relativistic flows, using Galilean transformations, by

$$V_1 = -(V'_1 - V_{sh}) = V_{sh} - V'_1, \quad (\text{C.1})$$

where the minus sign is included because for $V_{sh} > V'_1$ the upstream medium would appear to be flowing in the opposite direction in the rest frame of the shock. Applying the same transfor-

mation to the downstream flow speed V_2 yields

$$V_2 = V_{sh} - V'_2. \quad (\text{C.2})$$

The ratio of upstream to downstream flow speeds in the shock frame equals the shock compression ratio, defined as the factor by which the number density n changes across the shock. That is,

$$s = \frac{V_1}{V_2} = \frac{n_2}{n_1}. \quad (\text{C.3})$$

Substituting V_2 from Eq. C.3 into Eq. C.2, the downstream flow speed in the spacecraft frame can be written as

$$V'_2 = V_{sh} - V_1/s = \frac{V_{sh}(s - 1) + V'_1}{s}. \quad (\text{C.4})$$

Note that when $V_{sh} = 0$, the above expression reduces to V'_1/s . The downstream shock-frame speed similarly reduces to V'_1/s when $V_{sh} = 0$ and the sign transformation in Eq. C.1 is reversed. The flow speeds observed by spacecraft and the flow speeds in the shock frame are therefore equivalent for stationary shocks.

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