Simulation of the Solar Energetic Particle Event on 2020 May 29 Observed by Parker Solar Probe

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Abstract

This paper presents a stochastic three-dimensional focused transport simulation of solar energetic particles (SEPs) produced by a data-driven coronal mass ejection (CME) shock propagating through a data-driven model of coronal and heliospheric magnetic fields. The injection of SEPs at the CME shock is treated using diffusive shock acceleration of post-shock suprathermal solar wind ions. A time-backward stochastic simulation is employed to solve the transport equation to obtain the SEP time–intensity profile at any location, energy, and pitch angle. The model is applied to a SEP event on 2020 May 29, observed by STEREO-A close to ~1 au and by Parker Solar Probe (PSP) when it was about 0.33 au away from the Sun. The SEP event was associated with a very slow CME with a plane-of-sky speed of 337 km s⁻¹ at a height below 6 Rs as reported in the SOHO/LASCO CME catalog. We compute the time profiles of particle flux at PSP and STEREO-A locations, and estimate both the spectral index of the proton energy spectrum for energies between ~2 and 16 MeV and the equivalent path length of the magnetic field lines experienced by the first arriving SEPs. We find that the simulation results are well correlated with observations. The SEP event could be explained by the acceleration of particles by a weak CME shock in the low solar corona that is not magnetically connected to the observers.

Unified Astronomy Thesaurus concepts: Solar energetic particles (1491); Solar particle emission (1517); Solar coronal mass ejection shocks (1997)

1. Introduction

Solar energetic particles (SEPs) consist of electrons, protons, and heavy ions produced in association with solar eruptions that occasionally can reach up to GeV energies. They have been studied for several decades because they can be measured directly by particle detectors on spacecraft and indirectly by neutron monitors on the ground during ground-level enhancement events. Understanding the origin and transport of SEPs is of vital importance to space weather predictions since exposure to a large number of high-energy particles could pose a significant risk to spacecraft electronics and astronauts in space.

SEPs are believed to be produced by either magnetic reconnection in solar flares or particle acceleration at shocks driven by coronal mass ejections (CMEs). Historically, SEP events have been divided into impulsive SEP events associated with solar flares, and gradual SEP events whose particles are thought to be accelerated by CME-driven shocks. Gradual events have proton intensities that are usually more elevated and longer-lived than those observed in impulsive events. The lower particle intensities and energies typically observed in impulsive events are also characterized by enhanced ³He abundances (Balasubramanyan & Serlemitsos 1974), elevated electron to proton ratios, and high charge states of heavy ions (Reames 1999). Diffusive shock acceleration (DSA; e.g., Baring 1997) is commonly believed to be the main acceleration mechanism responsible for the particle energization in gradual events. Most gradual SEP events are associated with the occurrence of fast CMEs, whose shocks can form in the solar corona and propagate through the heliosphere. If the conditions are appropriate, the CME shocks can continuously accelerate particles as they propagate from their formation in the low corona and as they move outward in interplanetary space. The precise location of the site of particle acceleration by a propagating shock is uncertain. Observations of the early phases of CMEs (Balmaceda et al. 2022) suggest that the estimated speeds during the hyperinflation phase (in which the CME undergoes a rapid lateral expansion) can be sufficiently high to generate shocks and to accelerate particles in the low corona. In order to distinguish whether particles are accelerated close to the Sun, in the outer corona, or in interplanetary space, the study of a SEP event associated with a slow CME might help to localize this acceleration site, since such weak CMEs are not expected to continuously drive strong shocks in interplanetary space. Long et al. (2021) presented observations of energetic electron acceleration through measurements of Type III radio emissions associated with a very weak shock in the corona with an Alfvén Mach number of ~1.008–1.013 and shock speed of ~400–600 km s⁻¹. Observing SEP ions from weak CMEs at 1 au is difficult because weak CMEs are not expected to drive strong shocks able to accelerate particles with enough energy and intensity to be observed above the background of particle instruments and of galactic cosmic-ray intensities.

Although many spacecraft have expanded our ability to probe the properties of SEPs through in situ measurements and remote-sensing observations, reliable models to predict SEP radiation hazards are still lacking. Physics-based numerical
models for the propagation and acceleration of SEPs from their source to Earth can help the prediction of SEPs. Over the years, several simulation tools have been developed to study the propagation of SEPs (e.g., Heras et al. 1992; Kallenrode 1993; Bieber et al. 1994; Dröge 1994; Ng & Reames 1994; Heras et al. 1995; Ruffolo 1995; Kallenrode & Wilberenz 1997; Lario et al. 1998; Giacalone et al. 2000; Zank et al. 2000; Li et al. 2003; Ng et al. 2003; Rice et al. 2003; Lee 2005; Qin et al. 2006; Zhang et al. 2009; Dröge et al. 2010; Luhmann et al. 2010; Kozarev et al. 2013; Marsh et al. 2015; Hu et al. 2017; Zhang & Zhao 2017; Wisen et al. 2022). Closely relevant to this paper are the works by Zhang et al. (2009) and Dröge et al. (2010) that modeled the propagation of SEPs by solving the Fokker–Planck transport equation with stochastic processes in a three-dimensional (3D) interplanetary magnetic field, where the Parker model of the interplanetary medium is used. The Parker model describes reasonably well the undisturbed magnetic field and solar wind plasma in interplanetary space, but the magnetic field in the solar corona is far more complicated and dynamic, making it difficult to use a fixed configuration to describe it adequately. SEP production and propagation through the solar corona cannot be modeled without a model of magnetic field and plasma in this region. Recently, a data-driven coronal magnetic field configuration has been adopted by applying a potential-field source–surface (PFSS) model to synoptic magnetogram measurements (Zhang & Zhao 2017) obtained from a number of magnetographs such as NSO/GONG. On the other hand, in this model and most previous models, SEP production by CME shocks is an ad hoc input. For example, in some models energetic particles were injected with an assumed energy spectrum at a fixed radial distance in the corona. However, the production of SEPs by a propagating CME-driven shock is far more complicated. First, the CME shock can continuously accelerate particles at different radial distances as it moves away from the Sun. Second, the properties of the CME shock vary with time, radial distance, and along its front. Third, the shocks driven by CMEs vary significantly from event to event, and the inclusion of the shock as a mobile source of particles should be based as much as possible on observations. A SEP model for space weather predictions should consider the propagation of the CME shock through the corona and interplanetary medium as realistically as possible. In this paper, the SEP model calculation (Zhang et al. 2009) is extended by injecting source particles at the location of the shock front reconstructed from coronagraph observations using an ellipsoidal model (Kwon et al. 2014) that allows us to capture realistic CME shock conditions. We also include a SEP seed injection model to determine the particle intensity level from the input of shock properties.

Our newly developed SEP model is applied to an SEP event that occurred on 2020 May 29 and was observed both by Parker Solar Probe (PSP), a spacecraft getting closer to the Sun than ever before, and by STEREO-A in a ∼1 au orbit around the Sun. We compute the time profiles of the particle intensities observed by both spacecraft, derive the event-integrated particle energy spectrum, and estimate the path length of the magnetic field line experienced by the first arriving ions. We find that the simulation results are well correlated with observations. The flux of 2.2 MeV protons from the simulation

\[ \frac{\partial f}{\partial t} - \nabla \cdot (\kappa \nabla f) + (\nabla \cdot \mathbf{V}) f + \nabla \cdot (\nabla f) = \frac{\partial}{\partial \mu} \left( D_{\mu \nu} \frac{\partial f}{\partial \mu} + \frac{d}{dt} f \frac{\partial f}{\partial \mu} + \frac{d}{dt} f \frac{\partial f}{\partial p} \right) = Q_0, \]  

(1)

where the terms on the left-hand side come from particle transport mechanisms: cross-field spatial diffusion with a tensor \( \kappa_{\perp} \), streaming along the ambient magnetic field or average magnetic field direction \( \mathbf{b} \) with particle speed \( v \) and pitch-angle cosine \( \mu \), convection with the background plasma velocity \( \mathbf{V} \), particle gradient/curvature drift \( V_d \), pitch-angle diffusion with a coefficient \( D_{\mu \nu} \), focusing \( d/\partial t \), and adiabatic cooling \( d/\partial t \). On the right-hand side of Equation (1), the term \( Q_0 \) represents the source rate of particles from a seed population at energies much lower than those of the SEPs measured during a SEP event (see description below).

Under the adiabatic approximation, the drift velocity, focusing rate, and cooling rate may be calculated from the ambient magnetic field \( \mathbf{B} = \mathbf{b} \) and plasma velocity \( \mathbf{V} \) through

\[ V_d = \frac{e}{qB} \left\{ \frac{1 - \mu^2}{2} \frac{B \cdot \nabla B}{B^2} + \mu^2 \frac{B \times (\mathbf{B} \cdot \nabla) \mathbf{B}}{B^3} + \frac{1 - \mu^2}{2} \frac{B (\mathbf{B} \cdot \nabla \times \mathbf{B})}{B^3} \right\}. \]  

(2)

[5] https://gong.nso.edu/data/magmap/archive.html
\[
\frac{d\mu}{dt} = - \frac{(1 - \mu^2)\mathbf{v}}{2} \cdot \nabla \ln B + \frac{\mu(1 - \mu^2)}{2} \times (\nabla \cdot \mathbf{V} - 3\mathbf{b}\mathbf{b} : \nabla \mathbf{V}) - \frac{(1 - \mu^2)m}{p} (\mathbf{V} \cdot \nabla \mathbf{V}) \cdot \mathbf{b},
\]

where \( q \) and \( m \) are the charge and mass of the particles, respectively. The formulae for the terms in the first-order partial derivatives can be found in many previous publications (Northrop 1963; Isenberg 1997; Qin et al. 2004, 2006). The second-order partial derivative terms represent the effects of magnetic field turbulence. The equation is truncated up to the diffusion term as approximated in the standard quasi-linear theory. All the diffusion terms related to \( p \) are neglected, considering that the propagation speed of magnetic field turbulence, typically the Alfvén speed or fast-mode MHD wave speed, is much less than the speed of particles, and change in stochastic particle momentum caused by electric field fluctuations in the turbulence is much slower than the adiabatic cooling by the background solar wind plasma. If we assume that phases of magnetic field turbulence with a steeply decreasing power spectrum at different wavelengths are completely random or independent, then pitch-angle scattering and cross-field spatial diffusion become uncorrelated, yielding zero off-diagonal diffusion elements in the diffusion tensor (Jokipii 1966).

Like the Parker transport equation, the focus transport equation (Equation (1)) can be applicable to shock acceleration (le Roux & Webb 2012; Zuo et al. 2013a, 2013b). It is accurate when the particle velocities are much greater than the shock speed (Zhang et al. 2009). The focus transport equation can allow the particle distribution function to be very anisotropic, which is required for describing SEPs near the Sun or in the early phase of an SEP event. Protons above MeV energies accelerated by CME shocks in the low corona discussed in this paper are suitable for the focus transport equation.

We seek the solution to the transport equation to get the distribution of particles as a function of time, energy, and pitch angle at any particular heliospheric location. The equation is a time-dependent five-dimensional second-order (Fokker–Planck) partial differential equation in the phase space. Typical finite difference or finite element methods become impractical for this high-dimensional application. We use time-backward stochastic differential equations derived from the left-hand side of the Equation (1) to describe the motion of the particle guiding center and momentum (Gardiner 1985; Zhang et al. 2009):

\[
\frac{d\mathbf{x}}{ds} = \sqrt{2\kappa_{\perp}} \cdot dw(s) + (\nabla \cdot \kappa_{\perp} - v_0 \mu(s) \mathbf{b} - \mathbf{V}_0) ds,
\]

\[
\frac{d\mu}{ds} = \left[ -\frac{d\mu}{dt} + \frac{\partial D_{\mu\mu}}{\partial \mu} \right] ds + \sqrt{2D_{\mu\mu}} dw(s),
\]

where \( dw(s) \) is a Wiener process as a function of \( s \), which is the time running backward. \( dw(s) \) can be generated by random numbers from a Gaussian distribution with a standard deviation of \( \sqrt{ds} \). The simulation of stochastic processes starts at the location \( \mathbf{x} \), pitch-angle \( \mu \), momentum \( p \), and time \( t \) where the solution to the particle distribution function is sought, i.e., \( x(0) = x, \mu(0) = \mu, \) and \( p(0) = p \) at initial backward time \( s = 0 \) starting at the observation time \( t \).

An exact solution to Equation (1) for any location, momentum, pitch-angle cosine and time can be written as (Freidlin 1985)

\[
f(t, \mathbf{x}, p, \mu) = \left\{ \int_{\mathbf{s}_0}^{t} Q_0(t - s, \mathbf{x}(s), p(s), \mu(s)) ds \right\} + \left\{ f_x(t - \mathbf{s}, \mathbf{x}_e, p_e, \mu_e) \right\},
\]

where \( (\cdot) \) denotes the expectation of what is inside and \( f_x(t - \mathbf{s}, \mathbf{x}_e, p_e, \mu_e) \) is the boundary or initial value of the distribution function when the stochastic processes hit a boundary or the initial time (the subindex \( e \) refers to the first exit of the simulation). For our simulation of SEPs produced by CME shocks, \( f_x = 0 \) if we choose the initial time before the solar eruption and set the inner boundary at the solar surface and outer boundary at a large enough radial distance. Therefore, the solution to the transport equation (Equation (1)) is the expectation of the source injection rate integrated over time along backward stochastic trajectories. This is a major difference with respect to the work by Zhang et al. (2009), where a boundary condition at a given inner distance in the upper corona was assigned as a point for the injection of SEPs. We now run stochastic trajectories backward in time from the location, energy, and pitch angle where we want to calculate the particle intensity until CME initiation. Trajectories that encounter particle sources at shock crossings will contribute to the average. Many simulated trajectories do not encounter the shock, so we design a scheme to drive the simulated stochastic trajectories toward the shock by introducing an artificial drift. This can be achieved by substituting \( f_x \) by \( (1 + a\mu_s) f_x \) in the transport equation, where \( a \) is a tuning parameter and \( \mu_s \) is the cosine of pitch angle to the magnetic field line outward from the Sun. The increased probability toward particle source at the shock is compensated by an exponential decay or killing term that weighs on the average. See Zhang et al. (2009) for a detailed description of this methodology. We typically simulate \( 10^4 \text{–} 10^5 \) trajectories until a statistically significant number of useful trajectories or a small enough error bar (i.e., a relative error bar \( \sqrt{ff} \) of less than 10%) for the expected value has been achieved. The value of \( a \) does not affect the computation result once enough statistics are achieved, but it does influence how fast the result can converge in the computer simulation.

The seed particle source of SEPs \( Q_0 \) is typically of particles with energies much lower than those of the measured SEPs we intend to simulate. Contribution of the SEP seed particles to the averaging of the distribution function \( f \) in Equation (8) as a function of momentum \( p \) is through particle acceleration at the CME shock with the term containing \( dp/dt \) in the transport equation (Equation (1)) or stochastic differential equation.
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Because the simulation of stochastic particle transport processes and pc where (Equation 7)). The detailed processes of diffusive shock acceleration must be simulated in order to correctly capture the amount of acceleration and seed particle source injection. Acceleration of SEPs from the seed particles occurs on a small scale near the shock ramp. Simulation of such acceleration processes takes a huge amount of computation time, and thus becomes impractical for large-scale simulation of SEP production and transport.

We take an alternative approach to incorporate diffusive shock acceleration in this model. We note that the steady-state DSA solution provides a momentum distribution of particles given by a power law with a slope \( \gamma_s = 3R/(R - 1) \) determined only by the shock compression ratio \( R \) up to a cutoff momentum \( (p_c) \) independent of the particle diffusion coefficient (e.g., Drury 1983) and the large-scale shock geometry. It is unlikely that SEP transport on the large-scale heliospheric magnetic field will affect the local shock acceleration of particles below the cutoff momentum. Therefore, the particle distribution function at the shock is known as long as we know how many total seed particles have been injected at the shock location. We can move the term of particle acceleration at the shock front to combine with the seed source rate to get a new accelerated SEP injection rate as

\[
Q = Q_0 + \frac{dp}{dt_{sh}} \left( \frac{p}{p_{\text{inj}}} \right)^{-\gamma_s} \frac{df_{\text{sh}}(p < p_c)}{dp},
\]

where

\[
f_{\text{sh}} = f_{\text{sh}0} \left( \frac{p}{p_{\text{inj}}} \right)^{-\gamma_s} \quad \text{for} \quad p < p_c,
\]

and \( p_c \) and \( p_{\text{inj}} \) will be determined as described below (see Equations (12) and (15)). Once the shock acceleration term is combined with the source term, the gain of particle momentum during the shock passage is no longer included in the stochastic differential equation according to the correspondence between the Fokker–Planck equation and stochastic differential equation.

Note that the acceleration or cooling term in the transport equation away from the location of the shock front and above \( p_c \) is still left in the particle transport calculation, and its effects on the gain or loss of particle momentum are still followed by the simulation of stochastic particle transport processes. Because \( \frac{dp}{dt_{sh}} \) is a \( \delta \)-function on the shock surface, where the plasma and magnetic field properties are discontinuous, the rate of momentum change \( dp/dt \) is ambiguous, primarily due to the discontinuity in the magnetic field direction relative to the shock normal. We average the shock SEP injection over all particle pitch angles to avoid such ambiguity, assuming that the particle distribution at the shock front is isotropic. We have compared these results with a calculation using an anisotropic acceleration term, and we found that the difference is minimal, probably because the particles do cross the shock at pitch angles very close to an isotropic distribution. The isotropic assumption is justified because of the expected enhanced turbulence in the vicinity of a shock. So the accelerated SEP source rate can be written as follows:

\[
Q = Q_0 + \frac{1}{3}(V_2 - V_1)\delta(x - x_{sh})p \frac{df_{\text{sh}}}{dp},
\]

where \( V_1 \) and \( V_2 \) are plasma speeds relative to the shock upstream and downstream, respectively, and \( x_{sh} \) is the instantaneous shock location. \( Q \) replaces \( Q_0 \) in Equation (8) in the calculation of the solution to the particle distribution function. The integration of the \( \delta \)-function over time \( \delta(x - x_{sh})ds \) is called local time. We use Tanaka’s formula and Ito stochastic calculus up to the second order to calculate the differential local time for each shock crossing (e.g., Björk 2015). The particle accelerations are calculated at any location on the shock surface where stochastic particles hit when the shock condition is satisfied. The majority of particle acceleration takes place at the shock, and its effect has been represented by the addition of the accelerated SEP source injection. Short of shock acceleration along the backward simulated trajectories, the particles starting at the initial backward time with energies above 1 MeV will never decrease their energy enough to have a direct contribution from the seed particle population of typically a few keV. Essentially, \( Q_0 \) can be considered zero, but the seed particles contribute indirectly through the injection of accelerated SEPs at the shock, which is constrained by a power-law distribution according to the theory of diffusive shock acceleration. In this way, we can speed up the computation and incorporate the shock acceleration without simulating the entire acceleration process. It is correct as long as acceleration obeys the result of diffusive shock acceleration theory.

The cutoff momentum of the shock power-law distribution \( p_c \) can be determined by the amount of time available for diffusive shock acceleration \( t_{\text{acc}} \) (Drury 1983):

\[
t_{\text{acc}} = \int_{p_{\text{inj}}}^{p_c} \frac{3}{V_1 - V_2} \left[ \frac{\kappa_1}{V_1} + \frac{\kappa_2}{V_2} \right] \frac{dp}{p},
\]

where \( p_{\text{inj}} = mv_{\text{inj}} \) (see discussion on particle injection speed later) is the momentum of injected seed particles, and \( \kappa_1 \) and \( \kappa_2 \) are the particle diffusion coefficients upstream and downstream of the shock, respectively. Because typically \( \kappa_2 \ll \kappa_1 \), the upstream condition essentially determines the acceleration time. Note that when a large enough number of energetic particles are generated by the acceleration of a CME shock, the anisotropy of the upstreaming particles can generate waves due to its effect on plasma instability. These waves can, in turn, prevent particles from escaping the shock by pitch-angle scattering. This feature has only been partially applied by using the Bohm diffusion limit as \( \kappa_1 = v/(3qB_1) \) to calculate the shock acceleration of particle sources, where \( v \) is the particle speed, \( q \) is the particle charge, and \( B_1 \) is the upstream magnetic field strength. Because of the increasing diffusion with momentum, the acceleration time has little dependence on \( p_{\text{inj}} \) \( (\ll p_c) \). The cutoff momentum \( p_c \) can be determined through Equation (12) by setting \( t_{\text{acc}} \) to be equal to the shorter of the shock lifetime \( t \) since the onset of the CME eruption and the time for adiabatic particle energy loss in the background solar wind plasma \( t_{\text{loss}} = 3(\nabla \cdot V)^{-1} \), i.e., \( t_{\text{acc}} = \min(t, t_{\text{loss}}) \).

The coronal magnetic field covering the region from 1 \( R_S \) to 2.5 \( R_S \) is adopted into the SEP model by applying the PFSS model to observations of synoptic magnetograms (the first one after the eruption) (Zhang & Zhao 2017), where \( R_S \) is the solar
radius. The results do not change much with time-dependent synoptic magnetograms (Zhao & Zhang 2018). The computation of SEP transport is done in the reference frame corotating with the Sun, where the coronal magnetic field is stationary. Beyond 2.5 $R_S$, a Parker model of the heliospheric magnetic field with an empirical solar wind speed and density profile (Leblanc et al. 1998) is used. In the corotation frame, the tangential component of the plasma velocity is $-\Omega_S (r - 2.5 R_S)$, with $\Omega_S$ being the angular rotation speed of the Sun. This means that the solar wind begins to lose corotation at 2.5 $R_S$ and becomes nonrotating at large enough radial distances. The computation domain extends from the inner boundary at 1 $R_S$ to an outer boundary at a radial distance of 20 $au$, far enough that it does not affect the calculation result in the inner heliosphere unless an abnormally large mean free path is used. Both the inner and outer boundaries are absorptive boundaries, where the SEP distribution function is set to zero.

The sources of accelerated SEPs comove with the CME shock. The location, shape, and time propagation of the CME are taken from an ellipsoid model developed by Kwon et al. (2014). A 3D CME shock surface is reconstructed using EUV and white-light coronagraph images from instruments on STEREO, the Solar Dynamics Observatory, and the Solar and Heliospheric Observatory, which cover a radial range from a few $R_S$ to tens of $R_S$. Depending on the solar eruption, each event typically contains several time frames from multiple vantage points that allow an identification of the large-scale CME shock geometry and its propagation through the solar corona. Beyond the last frame, when the CME shock extends out of the field of view of the coronagraphs, a friction CME shock propagation model is adopted to model the slowdown of the CME shock. The radial distance of the shock front at the nose, $r_{shf}$, slows down according to

$$r_{shf} = r_{shf0} + V_{sw}(t - t_0) + \frac{V_{shf0} - V_{sw}}{b}(1 - e^{-b(t-t_0)}),$$  \hspace{1cm} (13)

where $r_{shf0}$ and $V_{shf0}$ are the initial radial distance and speed of the shock front at the nose as determined by fits to coronagraph observations, respectively, and $V_{sw}$ is the solar wind speed; $b$ in the dimension of $1/t$ is the parameter to measure the rate of shock slowdown. We use a parameter $t_{1au}$ to control the time when CME shocks pass 1 au and estimate the deceleration rate of the CME shock. We insert the ellipsoid shock surface and its time evolution into the coronal and heliospheric magnetic field and plasma configuration to derive the shock properties at any point on the shock surface. To numerically derive the fast-mode plasma compression ratio $R$ at the shock, relevant parameters, such as shock speed relative to the plasma, shock normal, plasma adiabatic index $\gamma$, upstream magnetic obliquity $\theta_{bn1}$, Alfvén Mach number $M_{A1}$, and fast magnetosonic Mach number $M_{MS1}$, are fed into the MHD shock adiabatic equation (e.g., Thompson 1962; Kabin 2001):

$$\begin{align*}
(1 - R \cos^2 \theta_{bn1} M_{A1}^{-2})^2 & \left[ (\gamma + 1 - \gamma R + R) - 2RM_{MS1}^{-2} \right] \\
- R \sin^2 \theta_{bn1} M_{A1}^{-2} & \left[ (2 - \gamma)R \right] \\
- (\gamma + 1 - \gamma R + R)R \cos^2 \theta_{bn1} M_{A1}^{-2} & = 0.
\end{align*}$$  \hspace{1cm} (14)

The downstream plasma density, velocity, magnetic field, and plasma thermal speed are further derived from the general jump conditions for oblique MHD shocks (Fitzpatrick 2014). Only a solution for a fast-mode shock is taken.

The shock compression ratio is used to determine the slope of the SEP power-law spectrum. We assume that particles are injected at the shock from the thermal tail of solar wind ions. The shock can substantially heat solar wind ions to become sub-magnetosonic after the shock crossing. Immediately downstream of the shock, the thermal tail particles have high enough energies to overcome convection away from the shock, and they are more likely to become the seed particles for diffusive shock acceleration. In this simulation, we choose a characteristic particle injection speed to be 2.5 times the shock speed, $v_{inj} = 2.5V_{sh}/\max (\cos \theta_{bn1}, 0.25)$. The term $1/\cos \theta_{bn1}$ is adopted since quasi-perpendicular shocks have a higher energy injection threshold than the quasi-parallel ones (Lee 2005; le Roux & Webb 2009). The number of injected seed particles can be related to the Maxwellian velocity distribution of downstream solar wind ions so that

$$f_{shf} = \frac{n_{sw2}}{(4\pi v_{sh2}^2)^{3/2}} \exp \left( -\frac{v^2}{2v_{sh2}^2} \right).$$  \hspace{1cm} (15)

where $n_{sw2}$ and $v_{sh2}$ are the downstream solar wind density and the thermal speed, respectively. The particle distribution function is illustrated in Figure 1, where a Maxwellian distribution and the resulting single power-law DSA distribution (see Equation (10)) are marked as the blue solid line and black solid line, respectively.

Because the choice of the injection speed sits in a Maxwellian tail, the total number of injected particles is sensitive to $v_{inj}$. We found that $v_{inj}$ between 2.3 and 2.7 $V_{sh}/\max (\cos \theta_{bn1}, 0.25)$ can generally produce a good fit to observations. Therefore, we set $v_{inj} = 2.5V_{sh}/\max (\cos \theta_{bn1}, 0.25)$ in this simulation. In addition, the code can handle arbitrary sources of seed particles. If a particular suprathermal population is injected, we can add the total number of injected particles to Equation (15).

Since the fitted ellipsoid shock is inserted into the plasma and magnetic field configuration obtained from the PFSS model, the downstream distribution of plasma and magnetic field inside the shock ellipsoid is not consistent with the shock jump condition. The calculation of particle acceleration is not entirely correct unless we modify the downstream magnetic field and plasma. This requires the input of a time-dependent plasma and magnetic field model. However, the effect of shock acceleration has been replaced by the injection of accelerated SEPs with a power-law spectrum determined by the shock compression ratio up to momentum $p_c$, so we do not have to correct for the change in plasma and magnetic field due to the CME shock propagation. For particles above $p_c$, the result still somewhat relies on calculating the shock acceleration process from a momentum below $p_c$, which is not an issue for most of our applications in this paper.

Our model also requires the input of particle transport coefficients, such as pitch-angle diffusion coefficient $D_{\mu\nu}$ and spatial diffusion perpendicular to the magnetic field $\kappa_z$. No direct measurements of these transport coefficients are possible. Their values can only be estimated through the spectrum of magnetic field turbulence with aid from a theory of particle transport coefficients. Alternatively, they can be treated as free parameters to fit observations. In this simulation, we follow an approach we have
adopted in a previous work (e.g., Zhang & Zhao 2017). We assign

\[ D_{ij} = D_0(r) \rho^{g-2} (1 - \mu^2) (|\mu|^{g-1} + h_0), \tag{16} \]

with \( q = 5/3 \) and \( h_0 = 0.2 \). The additional parameter \( h_0 \) is to phenomenologically describe the enhancement of scattering through \( \mu = 0 \) by either nonresonant scattering or nonlinear effects. The simulation assumes a constant radial particle mean free path \( \lambda_r \) of 10.0 \( R_s \) or 0.0465 au for particles of 1 GV rigidity with \( \lambda_r = 10R_s/p/1 \text{ GV}^{1/3} \). \( D_0(r) \) is chosen such that \( \lambda_r = \lambda_0 \cos^2 \psi \) with \( \lambda_0 = \frac{\sqrt{v}}{\pi} \int_0^1 d\mu (1 - \mu^2)^{1/2} \) (Hasselmann & Wibberenz 1970), where \( \psi \) is the spiral angle of the Parker magnetic field to the radial direction. Equation (16) is based on the quasi-linear theory of particle scattering by magnetic field fluctuations with a Kolmogorov spectrum, plus a nonlinear correction at the 90° pitch angle. The perpendicular diffusion is assumed to be mainly driven by field line random walk that starts at the bottom of the solar corona. A derivation by Zhang & Zhao (2017) yielded

\[ \kappa_\perp = \frac{v}{2V} k \kappa_{gd0} \frac{B_0}{B}, \tag{17} \]

where \( \kappa_{gd0} = 3.4 \times 10^{13} \text{ cm}^2 \text{ s}^{-1} \) is the diffusion coefficient in the photosphere estimated from a typical speed of supergranular motion, \( v/V \) is the ratio of particle speed to solar wind plasma speed, and \( B_0/B \) is the expansion of the magnetic field flux tube from the solar surface. A factor \( k \) is inserted to tune down the transmission of field line diffusion from the photosphere to the corona. In this simulation we set \( k = 0.074 \).

3. Results

We now apply our model calculation to the 2020 May 29 SEP event, one of the six SEP events observed during 2020 May 22–June 1 as described by Chhiber et al. (2021) and Cohen et al. (2021) (see also Zhuang et al. 2022). We choose to simulate this SEP event because the associated CME-driven shock can be reconstructed from coronagraph measurements. On 2020 May 29, PSP was at a heliocentric radial distance of 0.33 au (71.0 \( R_s \)). The involved active region (AR) was AR12764 at N34 in the northern hemisphere. A slow CME with a plane-of-sky speed estimated as 337 km s\(^{-1} \) at heights below 6 \( R_s \) has been reported in the SOHO/LASCO CME catalog7 (Yashiro et al. 2004; Gopalswamy et al. 2009).

The locations of PSP, Earth, and STEREO-A at 08:04 UT on 2020 May 29 are labeled by the letters P, E, and A in Figure 2(a), respectively, where the Sun is at the center. Sample magnetic field lines are shown as spiral curves, with the field lines passing through PSP shown as red curves. The blue arrow denotes the direction in which the CME headed (i.e., \( \sim 92° \) east in longitude from the Earth–Sun line). The reconstructed CME shock viewed from two different angles is indicated by the green surface in Figures 2(b) and 2(c), where the white sphere indicates the solar surface. STEREO-A was located 72° in longitude east of Earth and at a heliocentric radial distance of 0.96 au (the 1 au distance is indicated by the dashed circle in Figure 2(a)). PSP was 151° in longitude ahead of Earth. None of the spacecraft PSP, STEREO-A, and SOHO (this last near the Earth–Sun Lagrangian L1 point) established magnetic connection with the reconstructed CME shock via nominal Parker spiral interplanetary magnetic field lines.

\[ \text{https://cdaw.gsfc.nasa.gov/CME_list/index.html} \]
The CME on 2020 May 29 had a very low speed. Figure 3 shows the time evolution of the properties of the wave front at the leading point along the direction indicated by the blue arrow in Figure 2(b). Also shown are the time variation of the radial distance of the shock leading point (r_{lead}), the wave front speed relative to the upstream plasma (u_{i1}), the Alfvén speed (V_A), solar wind speed (V_{sw}), Alfvén Mach number (M_A = u_{i1}/V_A), fast magneto sonic Mach number (M_{MS}), shock compression ratio (R), and oblique angle (\theta_{ob}). The shock only exists in the radial distance range of around 1.7–2.5 R_S from 07:38 UT to 08:10 UT. Below 1.7 R_S, the wave front is slower than the Alfvén speed. Starting from the radial distance of 2.5 R_S or time 08:10 UT, the solar wind speed has increased enough so that the wave front speed relative to the plasma is less than the Alfvén speed. The shock cannot form below M_A = 1, and the compression ratio is set to 1. During the limited time period in which the shock exists, the maximum value of the compression ratio is \sim 1.6. The particles at the leading point undergo accelerations from a quasi-parallel shock as shown in Figure 3(e). Considering that the particle accelerations are calculated at the whole shock surface, accelerations from quasi-perpendicular shocks also exist at other positions on the shock surface. Since the CME shock only survives up to 08:10 UT below 2.5 R_S, the assumption about how the shock propagates or slows down at later time does not affect our result. Note that Figure 3 is only for the leading point (or apex) of the reconstructed shock. It is possible that other regions of the shock front, e.g., propagating in a medium with lower Alfvén speed, created a stronger shock.

In spite of the lack of magnetic connection between PSP and the CME shock, SEPs were seen to propagate to the location of PSP. Assuming that the SEPs observed by PSP were accelerated by the CME shock, one possibility for the particles to reach PSP is through particle diffusion across the nominal average interplanetary magnetic field lines. There is also the possibility that the interplanetary magnetic field configuration differed from the nominal field configuration shown in Figure 2(a) as pointed out in Appendix A of Zhuang et al. (2022), but this possibility will not be analyzed here because of the complexity and uncertainty of the exact magnetic field topology at the onset of the SEP event. Figure 4 shows the proton intensity–time profiles at two different energies observed by PSP (open symbols) and obtained by our simulations (solid traces). Observational data are from the EPI-Hi instrument, which measures energetic protons and heavy ions from \sim 1 to \sim 100 MeV/nucleon (McComas et al. 2016). Overall, the evolution of the proton flux from the simulation is well correlated with the observations. The flux of 2.2 MeV protons from the simulation and the observation are of the same order of magnitude with peak values of 0.32 (cm^2 s sr MeV)^{-1} and 0.15 (cm^2 s sr MeV)^{-1}, respectively. Observationally, the onset of the 2.2 MeV proton intensity enhancement occurred around 08:30 UT, whereas the simulated 2.2 MeV proton intensities increased 1.5 hr later. Such a delay can probably be shortened by fine-tuning both parallel and perpendicular mean free paths, but here we do not perform a parameter search due to the demand of computation time. The simulated 12 MeV proton intensities display a similar behavior to the observed intensities, with a delayed onset and a greater intensity. The peak intensities at both energies are within a factor of 2 of the observed values. At the current stage of research, fine-tuning these parameters will not be necessary because, among other factors, the uncertainty of the solar wind density of our plasma model can easily exceed a factor of 2.

Figure 5 shows the event-integrated energy spectra of the observed (blue) and simulated (red) SEPs. Observed and simulated spectra, marked as diamonds and circles, respectively, are calculated by integrating the ion flux over the time period 07:30–21:30 UT for all energetic particles below 20 MeV at PSP. The blue (red) line shows the power-law fit to the spectrum from PSP observation (simulation). The estimated spectral index is 2.08 from the simulation, which is consistent with the slope of 2.18 from the PSP observation (2.31 for all energetic particles up to 30 MeV in Cohen et al. 2021). Although a seed population is needed to start the particle acceleration and determine the particle intensity level, according to the diffusive shock acceleration theory, the shape of the energy spectrum is not sensitive to seed particle injection. The close match between the observed and simulated spectra indicates that diffusive shock acceleration can explain the SEP production in this event. The estimated energy spectral index of 2.08 corresponds to a momentum spectral index \gamma_s = 6.16. The compression ratio calculated from \gamma_s = 3R/(R - 1) should be 1.95, which is a little larger than the compression ratios obtained from the modeled shock structure as displayed in Figure 3. At a compression ratio of 1.60, the slope of the
The particle distribution function at the shock is expected to be 8. The slightly higher index of the observed event-integrated spectrum may result from energy-dependent particle propagation effects.

We also estimate the path length at the onset time from the plot of reciprocal particle velocity $1/v$ versus onset time in Figure 6. The onset time is chosen as the time when the flux
from the Solar Electron and Proton Telescope (SEPT; Müller-Mellin et al. 2008) on STEREO-A as shown by the blue dashed curve in Figure 7. To examine it, the time evolution of the simulated proton flux at STEREO-A for 1.5 MeV (blue solid curve) and 5.0 MeV (red solid curve) is shown in Figure 7. The simulated particle intensity is obtained with the same model setup as was used to simulate for the locale of PSP. The modeled flux of 5.0 MeV protons has a peak value around $3.6 \times 10^{-3} \text{cm}^{-2} \text{s}^{-1} \text{sr}^{-1} \text{MeV}^{-1}$, which is between the peak value of the 1.8–3.6 MeV (green dashed curve) and 4.0–6.0 MeV (red dashed curve) proton intensities measured by the LET (Mewaldt et al. 2008) on STEREO-A and much larger than the background fluxes of $\sim 1 \times 10^{-4} \text{cm}^{-2} \text{s}^{-1} \text{sr}^{-1} \text{MeV}^{-1}$ of 4.0–6.0 MeV protons and $\sim 4.0 \times 10^{-4} \text{cm}^{-2} \text{s}^{-1} \text{sr}^{-1} \text{MeV}^{-1}$ of 1.8–3.6 MeV protons. However, the predicted flux of 1.5 MeV protons from our simulation peaks at around 0.03 (cm$^2$ s sr MeV)$^{-1}$, which is smaller than the background ion flux of $\sim 0.07 \text{cm}^{-2} \text{s}^{-1} \text{sr}^{-1} \text{MeV}^{-1}$ of 1.11–1.98 MeV protons from STEREO-A/SEPT. Thus, this explains why no clear enhancement of 1.11–1.98 MeV protons was seen by STEREO-A/SEPT. Low-energy particles have mean free paths that are too short to reach 1 au before they dissipate in interplanetary space through adiabatic cooling. The peak intensity of high-energy protons at 5.0 MeV is comparable to the predicted peak level in our simulation without adjusting the model parameter from the runs for PSP. The rise in the 4.0–6.0 MeV proton flux appears later than the prediction, suggesting that the particle mean free path between 0.33 and 1 au needs to be adjusted to a slightly lower value.

Our calculations for SOHO do not show any SEP fluxes above the background level of the instrument on this spacecraft. The result is consistent with the observation of no SEP enhancement during the time period.

### 4. Summary and Discussion

In this paper, a simulation has been carried out using time-backward stochastic differential equations to derive energetic particle intensities during SEP events from the focus transport equation. A SEP source term is given in a form consistent with the theory of diffusive shock acceleration by a CME shock front. It only needs an input of the particle distribution function of accelerated SEPs at the shock front, which can be established once the local shock compression is known and the total number of injected particles is estimated. The code takes the input of the coronal magnetic field configuration based on a data-driven PFSS model and propagates a CME shock reconstructed from coronagraph observations. The simulation is applied to the 2020 May 29 SEP event observed by PSP, while PSP was not magnetically connected to the CME shock. We calculate the proton intensity–time profile at PSP and estimate the spectral index of ions between $\sim 2$ and 16 MeV and the path length of the field line experienced by particles at the event onset. Overall, our results are consistent with the observations. The fluxes of 2.2 MeV protons from the simulation and the PSP observation are of the same order of magnitude with peak values of 0.32 (cm$^2$ s sr MeV)$^{-1}$ and 0.15 (cm$^2$ s sr MeV)$^{-1}$, respectively, whereas the simulated 2.2 MeV proton intensity increased 1.5 hr later than that from the PSP observations. The modeled flux of 5.0 MeV protons has a peak value around $3.6 \times 10^{-3} \text{cm}^{-2} \text{s}^{-1} \text{sr}^{-1} \text{MeV}^{-1}$, which is between the peak values of the 1.8–3.6 MeV and 4.0–6.0 MeV proton intensities measured by the LET on STEREO-A. The

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**Figure 6.** Path length at the onset time estimated from the plot of reciprocal particle velocity $1/\nu$ vs. time from the simulation. The red dashed line shows a least chi-square linear fit line with a slope around 1.43 au$^{-1}$, which corresponds to a path length of $\sim 0.70$ au.
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**Figure 7.** Time evolution of proton flux at 1.11–1.98 MeV (blue dashed curve), 1.8–3.6 MeV (green dashed curve), and 4.0–6.0 MeV (red dashed curve) from STEREO-A observations and the proton flux at 1.5 MeV (blue solid curve) and 5.0 MeV (red solid curve) from the simulation. Data of the observations are from the LET and SEPT instruments of STEREO-A.

estimated spectral index is 2.08 from the simulation, which is consistent with the slope of 2.18 from the PSP observation. The estimated equivalent path length of 0.70 au is slightly longer than 0.625 au from the PSP observations estimated by Chhiber et al. (2021). Even though the CME is slow, below the speed of the fully accelerated solar wind, it could drive a shock wave and accelerate particles in the low solar corona. Because the heliocentric radial distance of PSP was small and, in principle, a shock driven by a slow CME can only survive in the low corona before the CME sufficiently expands, the probability of a direct magnetic connection between a spacecraft and a mobile source of particles through the average magnetic field is quite low. The fact that SEPs were seen by PSP requires the particles to propagate across magnetic field lines. A rate of about 10% supergranular diffusion for the field line random walk is assumed in this paper to drive the particles’ perpendicular diffusion (Zhang & Zhao 2017). If the perpendicular transport of particles is through the random walk of magnetic field lines, we found that a fraction of supergranular diffusion at the base of the photosphere is sufficient to explain the particle diffusion that is needed for PSP observations.

The injection of seed particles for shock acceleration still needs fundamental understanding since the theory is rather vague. In reality, the seed injection depends very strongly on the magnetic field configuration and the populations of thermal and suprathermal particles near the shock. There is little information about them in the solar corona, and it is probable that their properties could change significantly depending on solar conditions or even solar events. If this is the case, then the calculation of the absolute level of SEP intensity may suffer significant uncertainty. Note that the simulation described above does not apply to SEP electrons because the gyroradii of particles should be much larger than the shock ramp for diffusive shock acceleration. However, the gyroradii of electrons up to several MeV are much smaller than those of ions and may not satisfy this condition. The values of particle injection speed $V_{\text{inj}}$ and tuning factor $k$ could significantly change the flux of protons. Though the flux level is sensitive to $V_{\text{inj}}$, a lower or higher $V_{\text{inj}}$ would not change the particle spectral shape for the single power-law portion that we are studying in Figure 5. In addition, it might be possible that the flux is overestimated for a slow CME shock in the low corona because of the relatively low injection speed we are using for the quasi-parallel portion of the CME shock. Parallel and perpendicular mean free paths can also affect the result. They can influence the peak intensity and location somewhat. However, if they are changed by an order of magnitude, the spectrum only goes up or down slightly. The values used in this paper seem to be a good fit for the 2020 May 29 SEP event. We do not believe they are kept the same for other SEP events. More work in future is needed to investigate this.

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