Chapter 3
Methodology of Fitting

An appropriate transport equation for particles released from the Sun (as mentioned in the previous chapter) was solved by the finite-difference method.

3.1 Simulation of the Interplanetary Transport of Solar Energetic Particles

The simulation program considers the effects of pitch-angle scattering, focusing, deceleration and convection by solving equation (2.37). The distribution function $F(t, \mu, z, p)$ depends on t (time), μ (the cosine of the pitch-angle), z (the distance along the magnetic field from the Sun), and p (the momentum of a particle). We split the right hand side of the transport equation (2.37) into individual terms and study the evolution of the particle distribution from $F(t, \mu, z, p)$ to $F(t + \Delta t, \mu, z, p)$ following these steps:

1. We study the effects of the μ-flux, related to pitch-angle scattering, focusing, and differential convection from μ to $\mu + \Delta\mu$. The μ-flux is given by

$$S_\mu(t, \mu, z, p) = \left[\frac{v}{2L(z)}\left(1 + \mu\frac{v_{sw}}{v}\sec\psi - \mu\frac{v_{sw}v}{c^2}\sec\psi\right)(1-\mu^2) \right.$$
$$\left. - v_{sw}\left(\cos\psi\frac{d}{dr}\sec\psi\right)\mu(1-\mu^2)\right] F(t, \mu, z, p)$$
$$-\frac{\varphi(\mu)}{2}\frac{\partial}{\partial\mu}\left(1 - \mu\frac{v_{sw}}{c^2}v\sec\psi\right) F(t, \mu, z, p). \qquad (3.1)$$

We constrain $\varphi(\mu = \pm 1)$ to zero, so that $S_\mu(\mu = \pm 1) = 0$ and particles will not flow or diffuse into the unphysical region $|\mu| > 1$. The numerical method we used changed the distribution function, F, according to

$$F(\mu) \leftarrow F(\mu) - \left(\frac{\Delta t}{4n}\right)\left[\frac{S_\mu(\mu+\Delta\mu/2) - S_\mu(\mu-\Delta\mu/2)}{\Delta\mu}\right] \tag{3.2}$$

$$F(\mu) + \left(\frac{\Delta t}{4n}\right)\left[\frac{S_\mu(\mu+\Delta\mu/2) - S_\mu(\mu-\Delta\mu/2)}{\Delta\mu}\right] \leftarrow F(\mu), \tag{3.3}$$

where n is the integer number of times the process is repeated. The error of this step is checked by repeating with shorter time steps (i.e., greater n) until the result changes less than the specified tolerance.

2. We study the effects of deceleration (a systematic decrease in momentum, p.) We use the equation for the deceleration part of transport as

$$\frac{\partial}{\partial t}F(t,\mu,z,p) = \frac{1}{\tau_d}\frac{\partial}{\partial p}pF(t,\mu,z,p), \tag{3.4}$$

where the deceleration time is

$$\frac{1}{\tau_d} = v_{sw}\left[\frac{\sec\psi}{2L(z)}(1-\mu^2) + \cos\psi\frac{d}{dr}\sec\psi\mu^2\right]. \tag{3.5}$$

We get

$$\frac{\partial}{\partial t}pF(t,\mu,z,p) = \frac{1}{\tau_d}\frac{\partial}{\partial \ln(p/p_0)}pF(t,\mu,z,p), \tag{3.6}$$

and

$$pF(t+\Delta t,\mu,z,p) = pe^{\Delta t/\tau_d}F(t,\mu,z,pe^{\Delta t/\tau_d}), \tag{3.7}$$

where $F(t,\mu,z,pe^{\Delta t/\tau_d})$ is found by geometric interpolation between p-grid points at time, t.

3. We study the effects of streaming and convection of particles from one z-grid point to another. From the equation for streaming and convection of particles, i.e., the transport equation with only those terms on the right hand side,

$$\frac{\partial F(t,\mu,z,p)}{\partial t} = -\frac{\partial}{\partial z}\mu v F(t,\mu,z,p) - \frac{\partial}{\partial z}\left(1-\mu^2\frac{v^2}{c^2}\right)v_{sw}\sec\psi F(t,\mu,z,p). \tag{3.8}$$

In previous work, when the distribution function was moved from one z-grid point to another in integral increments of Δz. However, the method yielded an irregular distribution function and required a very small Δz, so it used a long run time. Now Nutaro et al. (2001) have developed a generalized total variation diminishing (TVD) method for this step. We use the generalized TVD method with equation (3.8), written in the form

$$\frac{\partial F(t,\mu,z,p)}{\partial t} = -\frac{\partial\left[v_z F(t,\mu,z,p)\right]}{\partial z}, \tag{3.9}$$

where

$$v_z = \mu v + \left(1 - \mu^2 \frac{v^2}{c^2}\right) v_{sw} \sec\psi F(t,\mu,z,p) \tag{3.10}$$

is the spatial velocity of the particles. The TVD method is an efficient numerical method that limits the amount of numerical diffusion and avoids oscillations by not creating any new minima or maxima in a given step. A TVD method was first presented by Harten 1983. The principle of TVD is

$$TV(F^{n+1}) \leqslant TV(F^n), \tag{3.11}$$

in which TV is the total variation of a function $F(x)$, defined by $TV = \int |\partial F/\partial x| dx$. This expression has a numerical (finite difference) form of $TV(F^n) = \sum_i |F^n_{i+1} - F^n_i|$, where i and n are spatial and time indices, respectively.

The usual TVD methods limit the Courant number, $\gamma = v_z \Delta t/\Delta z$, to $0 \leqslant \gamma \leqslant 1$. However, we would like the freedom to set Δz to a higher value, which may lead to improved accuracy, although the condition of $\Delta z > v_z \Delta t$ may decrease the speed of the algorithm. Therefore, we want to able to set $\gamma > 1$ and vary γ with position, too. This was the motivation for the generalized TVD algorithm (Nutaro et al. 2001).

We consider that the distribution function, F, is first moved by an integral number of steps, g (e.g., F is moved from point $l-g$ to l) and then we consider the remainder by defining $\gamma' = \gamma - g$, with $0 \leqslant \gamma' < 1$, so

$$F_l = F_{l-g} - \frac{\Delta t}{\Delta z}\left[S'_{l+1/2} - S'_{l-1/2}\right], \tag{3.12}$$

where $S'_{l+1/2}$ is the flux of particles from z-grid point l to $l+1$ due to γ'. $S'_{l+1/2}$ is defined as

$$S'_{l+1/2} \equiv v'_{l+1/2}F_{l-g} + \frac{1}{2}v'_{l+1/2}\left(1-\gamma'_{l-1/2}\right)\left(F_{l-g+1} - F_{l-g}\right)\varphi_l, \tag{3.13}$$

where φ_l is the flux limiter (Roe 1985). One can prove the consistency of the generalized TVD method by using Taylor series expansions. The convergence can be to first or second order in Δz (Nutaro et al. 2001).

These main steps are developed for use in simulating the transport of solar energetic particles in the program, "wind." This program will get the initial values for simulating the event of interest from the user to calculate basic variables and call other files (each file solves a different part of the transport equation) to run for specific cases.

We compile and link this program by calling other files. Some files have several versions. We select the appropriate version for the transport problem of interest. The simulation gives the particle distribution as a function of time and energy for each choice of the mean free path.

We examine the characteristics of the energetic heavy ions from solar events of interest by comparing results from this simulation program with the data from spacecraft. We use techniques for data fitting, including the linear least squares method, as we will discuss in the next section.

3.2 Least Squares Fitting

The simulation gives the particle distribution function vs. time. The spacecraft or ground-based data include the intensity and/or anisotropy of particles vs. time and their uncertainties. We use the techniques of linear least squares and a piecewise linear injection function, along with our transport simulation results and optimization of the injection onset and duration, to fit the data. This type of problem can be called an inversion problem. We choose a general, linear form of the fitting function:

$$\hat{y}(x) = \sum_{k=1}^{M} a_k X_k(x), \tag{3.14}$$

where $X_1(x), \ldots, X_M(x)$ are arbitrary fixed functions of x, $\{a_k\}$ are the parameters to be fitted and M is the number of fixed functions. The χ^2 value expresses the difference between the results from the simulation program and the spacecraft or ground-based data and is defined as

$$\chi^2 = \sum_{i=1}^{N} \left[\frac{y_i - \sum_{k=1}^{M} a_k X_k(x_i)}{\sigma_i} \right]^2, \tag{3.15}$$

where (x_i, y_i) is the ith data point from the spacecraft or ground-based data, σ_i is the error of the ith data point, and N is the number of data points. We minimize χ^2 by adjusting parameters in the model, which are choosing the appropriate injection function (in this work we use the piecewise linear injection function as discussed in the next section) and using the accurate uncertainties of the data (σ_i), as discussed in section (3.4). We find the parameters that give the best fit to the data by setting:

$$\frac{\partial \chi^2}{\partial a_1} = 0$$

$$\begin{aligned} \frac{\partial \chi^2}{\partial a_2} &= 0 \\ &\vdots \\ \frac{\partial \chi^2}{\partial a_k} &= 0. \end{aligned} \tag{3.16}$$

From equation (3.12), we get

$$0 = \sum_{i=1}^{N} \frac{\left[y_i - \sum_{j=1}^{M} a_j X_j(x_i)\right]}{\sigma_i^2} X_k(x_i), \quad k = 1, \cdots, M. \tag{3.17}$$

Finally, we get the values of $\{a_j\}$ from solving the matrix equation

$$\sum_{j=1}^{M} \alpha_{kj} a_j = \beta_k, \tag{3.18}$$

in which

$$\alpha_{kj} = \sum_{i=1}^{N} \frac{X_j(x_i) X_k(x_i)}{\sigma_i^2}, \tag{3.19}$$

and

$$\beta_k = \sum_{i=1}^{N} \frac{y_i X_k(x_i)}{\sigma_i^2}. \tag{3.20}$$

If the minimum $\chi^2/d.f.$ is close to 1, that indicates a good fit, where $d.f.$ is the number of degrees of freedom, i.e., the number of data points minus the number of parameters. If $\chi^2/d.f.$ is much larger than 1, this indicated a poor fit, but if $\chi^2/d.f.$ is much less than 1, it probably has too many parameters or has too large error estimates (σ_i).

The results from the simulation program are the particle distribution function vs. time for various λ values that result from a delta-function (instantaneous) injection. We thus know the response function for the injection near the Sun at a single instant in time. We model the injection function versus time near the Sun as a piecewise linear function.

3.3 Piecewise Linear Injection Function

We use specially developed techniques to deconvolve the effects of interplanetary transport for determining the injection profile near the Sun, in which the best-fit values with the appropriate mean free path, λ, together give the injection function. We have an "inversion problem,"

$$R(t) = \int_0^\infty G(t-t')I(t')dt', \tag{3.21}$$

where $I(t')$ is the injection of particles versus time near the Sun, $G(t-t')$ is the Green's function, or the response to a delta-function injection, and $R(t)$ is the response function, i.e., the intensity or anisotropy measured by an observer near the Earth.

Our method finds the optimal piecewise linear injection function, $I(t')$, for a set of "joint times," t_i, In general, a piecewise linear function is a linear combination of triangular functions (Mathews et al. 1999, Pinsky 1998, Atkinson 1989), $I_i(t')$. The profile of each triangular function starts from no injection at the start time, rising linearly to a peak injection of 1 at the peak time, and declining linearly to 0 at the end time. This peak time is the start time of the next function, and the end time becomes the peak time of the next function, as seen in Figure (3.1a).

We convolute $G(t-t')$, the transport simulation result for an instantaneous injection, with each $I_i(t')$, giving the response function, $R_i(t)$, in Figure (3.1b) due to each triangular injection. Thus the total response function, $R(t)$, is a linear combination of $\{R_i(t)\}$ (Figure 3.1d). Because the transport equation (2.37) is linear in $F(t, \mu, z, p)$, the response function, $R(t)$, that corresponds to a linear combination of triangular injection functions, $I(t') = \sum_i a_i I_i(t')$, (Figure

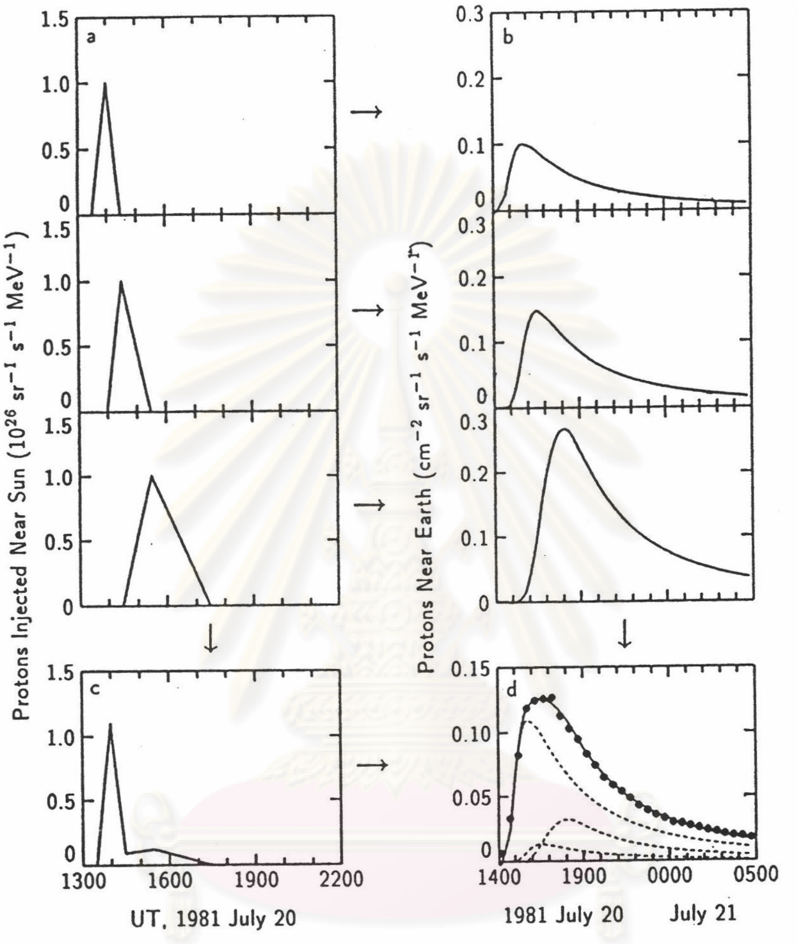

Figure 3.1: The deconvolution technique for a piecewise linear injection function near the Sun: a) shows the triangular injection profiles, b) shows the response functions, which result from the convolution of the Green's function with each triangular injection profile from a), c) is the best-fit piecewise linear injection profile, and d) is the linear combination (solid line) of response functions (dashed lines).

3.1c), is the same linear combination of each response function, $R(t) = \sum_i a_i R_i(t)$ (Figure 3.1d). Finally, we find the best piecewise linear injection function, $I(t')$, from the set of coefficients, $\{a_i\}$, which give the best-fit result between $R(t)$ and the spacecraft or ground-based data.

These relations concern our technique for fitting in that we can use linear least-squares fitting to find the linear combination that minimizes the χ^2 value between $R(t)$ and the data. Each triangular injection $I_i(t')$ has a peak of value of 1, which is multiplied by the coefficient a_i. The coefficient a_i is thus the value of the injection function at each peak time.

We use the results from the simulation program, the spacecraft data and the set of joint times (see next section) as the input file for the fitting program. If the starting time point of the rise of the fitting function is not the same as the start time of the rise toward the peak in the data, then we can shift the start time in the file of the set of joint times to the appropriate time (Ruffolo, Khumlumlert, and Youngdee, 1998). So far we have described a deconvolution technique to find the optimal piecewise linear injection function for a given set of joint times. We will discuss the new development of a method to set the joint times in the following section.

3.4 Automatic Truncation of the Injection Function and Variation of Joint Times

In the previous section we described a deconvolution technique to find the optimal piecewise linear injection function for a given set of "joint" times. In previous work, one would input the set of joint times for the piecewise linear injection function. In the present work, we have developed a new technique for setting the joint times, as well as an automatic truncation of the piecewise linear injection function.

We set the joint times of the piecewise linear injection function to be

$$t_\circ = t_{flare} + \delta \tag{3.22}$$

and

$$t_i = t_\circ + 2^{(i-1)}\ \varepsilon\ dt, \tag{3.23}$$

where dt is the time spacing of the data, and (δ, ε) are optimized automatically, with a simple regularly spaced search pattern, performed first for a coarse and then a finer spacing. Note that $t_\circ$ is the start time of the injection, and we set the t_i's (later times) within the pulse data range. The last t_i is the first value beyond the second half-maximum point of the data. This method is more systematic, flexible, and automated than that of Ruffolo, Khumlumlert, and Youngdee (1998).

The truncation algorithm that is automated in the present work was described by Ruffolo, Khumlumlert, and Youngdee (1998), who manually set the joint times in the least squares fitting based on the χ^2 value between the simulation results and the collected data. For a given set of joint times, i.e., given δ and ε values, the least squares fitting yields the coefficients a_i representing the values of the injection function at time and σ_i, the statistical error of each a_i. We truncate by removing the last joint time if any of the fitting coefficients, $\{a_i\}$, are negative (unphysical), or if the last coefficient is not greater than $2\sigma_i$ (i.e., not significantly different from zero). Then we cut the last joint time and refit the data again.

From the automatic fitting program, we get the fitting result between the spacecraft or ground-based data and the convolution of transport simulation

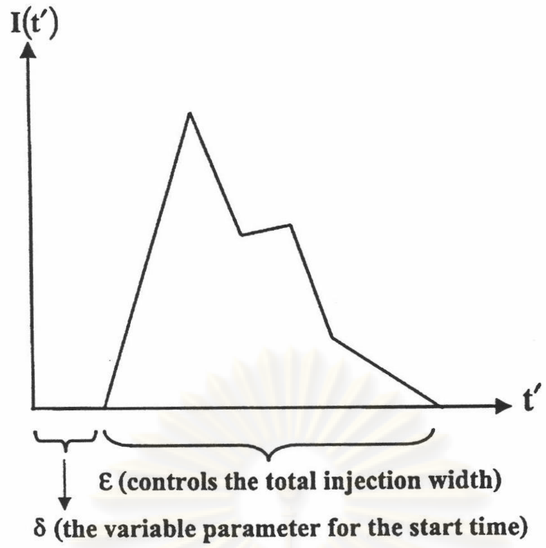

Figure 3.2: Example of joint times of the injection function, determined by ϵ and δ.

results with the best-fit injection function, for each mean free path. The fitting results give the details about χ^2, ϵ, δ, $\{a_i\}$ and their uncertainties, determining the injection function.

3.5 Procedure for the Fitting

The author used the technique of a finite difference method to solve the transport equation (Ruffolo 1995). We used the simulation program for fitting various solar flare events. We further developed some routines corresponding to the events that we chose to study, e.g., changing some defined values or modifying some parts of the program to get the desired simulation results.

The results from the simulation program are the particle intensity and/or anisotropy for various mean free paths that result from a delta-function injection. We thus know the response function for an injection near the Sun at a single instant in time. The injection function versus time near the Sun is modeled as a piecewise linear function, as a sum of triangular functions (Ruffolo, Khumlumlert, and Youngdee, 1998). The output from the simulation program consist of 2 columns. The first column is time in minutes and the second column is the intensity of particles in units of 10^{28} $sr^{-1}s^{-1}MeV^{-1}$. We want to fit the simulation results to the spacecraft or ground-based data by finding the optimal injection function. The data file consist of 3 columns: the first column is the time in minutes, the second column is the flux or the anisotropy$\times$intensity of the particles, and the third column is the uncertainty (discussed in more detail in the next chapter). We must input the initial values for the automated fitting program relying on the linear least squares technique. Those initial values are:

1. The background value of the spacecraft data, before the start of the solar event.
2. The estimated start time of the event.
3. The time at half maximum after the peak of the spacecraft data.
4. The time interval width of the data.
5. The start value for ε.
6. The $\Delta\varepsilon$ value.
7. The number of ε values.
8. The "standard" value of ε.
9. The start value for δ.
10. The $\Delta\delta$ value.
11. The number of δ values.

We used the output of the simulation, representing the response to the delta-function injection for each mean free path, convoluted with each automatically truncated and optimized triangular injection function to produce the fitting

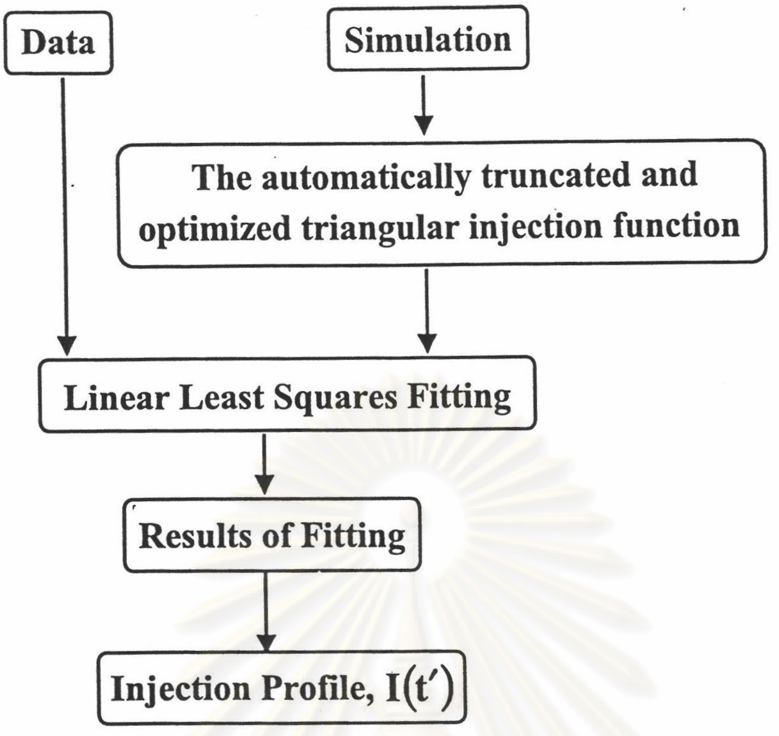

Figure 3.3: Flow chart of the fitting method

function for the linear least squares program. The program fits the spacecraft or ground-based data with an automated linear combination of fitting functions to find the coefficients $\{a_i\}$ that describe the injection of the solar energetic particles at each joint time. Finally we get the best piecewise linear injection and χ^2 value for each mean free path. The fitting result that has the minimum χ^2 is the best fit. We summarize the fitting method for finding the injection function as in the flow chart of Figure 3.3.

We find the error of the estimated mean free path by plotting the parabolic curve of 3 points (λ, χ^2) from the 3 best fits performed. We identify λ at the minimum χ^2 among the fits performed (λ_{fit}). We get the minimum χ^2 value from the parabolic curve λ vs. χ^2, and we set λ at the minimum point of the graph to be λ_{best} and also derive the χ^2 value (χ^2_{best}) for λ_{best}. We find $\Delta\lambda$ by finding

$\lambda \pm \Delta\lambda$ which have the χ^2 value in the parabolic fit equal to the χ^2_{best} +1.

We find the duration of the injection of solar energetic particles from the fitting results. The fitting results report the injection coefficient a_i at each joint time of the piecewise linear injection function. We express the injection duration of the event in terms of the full width at half maximum of the injection function. From this fitting method, we obtain our estimate of the mean free path, $\lambda_{best} \pm \Delta\lambda$, the optimal χ^2 value, χ^2_{best}, the injection duration, and a file comparing the best-fit response function and the spacecraft or ground-based data vs. time and their uncertainties. Examples of such summary results are given in Appendix C.