The influence of pickup protons, from interstellar neutral hydrogen, on the propagation of interplanetary shocks from the Halloween 2003 solar events to ACE and Ulysses: A 3-D MHD modeling study

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We describe our 3-D, time-dependent, MHD solar wind model that we recently modified to include the physics of pickup protons from interstellar neutral hydrogen. The model has a time-dependent lower boundary condition, at 0.1 AU, that is driven by source surface map files through an empirical interface module. We describe the empirical interface and its parameter tuning to maximize model agreement with background (quiet) solar wind observations at ACE. We then give results of a simulation study of the famous Halloween 2003 series of solar events. We began with shock inputs from the Fearless Forecast real-time shock arrival prediction study, and then we iteratively adjusted input shock speeds to obtain agreement between observed and simulated shock arrival times at ACE. We then extended the model grid to 5.5 AU and compared those simulation results with Ulysses observations at 5.2 AU. Next we undertook the more difficult tuning of shock speeds and locations to get matching shock arrival times at both ACE and Ulysses. Then we ran this last case again with neutral hydrogen density set to zero, to identify the effect of pickup ions. We show that the speed of interplanetary shocks propagating from the Sun to Ulysses is reduced by the effects of pickup protons. We plan to make further improvements to the model as we continue our benchmarking process to 10 AU, comparing our results with Cassini observations, and eventually on to 100 AU, comparing our results with Voyager 1 and 2 observations.


1. Introduction

Data beamed back to Earth by the Voyager 1 and 2 spacecraft from the fringe of our heliosphere offer us an opportunity to test and improve our understanding of this dynamic and complex region near the outskirts of our neighborhood in space.

The spherically expanding solar wind comes into pressure balance with the local interstellar medium (LISM) through the termination shock (TS) which greatly reduces the solar wind speed. Pressure fluctuations in the turbulent solar wind make the location of the termination shock highly dynamic; it moved across Voyager 2 five times [Richardson et al., 2008; Burlaga et al., 2008; Intriligator et al., 2010a, 2010b]. Pressure variations resulting directly from solar activity include interplanetary shock waves, coronal mass ejections (CMEs), corotating interaction regions (CIRs), and global merged interaction regions (GMIRs). While both Voyager spacecraft were still inside the TS, they both observed very large pressure variations associated with the Halloween 2003 series of solar events.

The LISM contains neutral hydrogen atoms that drift unperturbed through the heliosheath and TS into the heliosphere. As this neutral hydrogen approaches the Sun, it begins to ionize by charge exchange with solar wind protons and through photoionization. These pickup protons transfer momentum and energy into the solar wind. Due to their high relative velocities, they slow and heat the solar wind. Heavier neutral atoms are also present in the LISM and become pickup ions, but we will not discuss them here.

Our broad goal is to validate this new model, consistent with its simplicity. That is, to benchmark our progress in understanding and modeling the solar wind and the propagation of solar disturbances to the outer heliosphere. And, our specific goal is to study the evolution of the...
Halloween 2003 storm chain disturbances as they propagate to the ACE, Ulysses, Cassini, Voyager 1, and 2 spacecraft. An important aspect for both goals is the influence of pickup protons on the solar wind flow, and on shock propagation. Toward these goals, we have added the basic physics of pickup protons (as mentioned above) to the Hybrid Heliospheric Modeling System (HHMS) ([Detman et al., 2006], a time-dependent three-dimensional (3-D) magnetohydrodynamic (MHD) solar wind model. The purpose of this paper is to describe the modified model, HHMS-PI, and to describe our initial results in simulating the propagation of the Halloween 2003 solar events to ACE and Ulysses. We expect to continue improving the model as we progress outward.

[6] An important and distinguishing feature of our model is that it has a dynamic time-dependent lower boundary condition close to the Sun (0.1 AU) that is driven through an empirical interface by solar photospheric, coronal, X-ray, and radio observations.

[7] We take a step-by-step approach, beginning with the tuning of empirical model parameters to make the model agree with the background solar wind at ACE. Then we move to the Halloween 2003 solar events, and introduce shock input perturbations. We iteratively adjust the shock inputs, first to match ACE observations, then we extend the grid and compare model results with Ulysses observations, near 5 AU. Next we use both ACE and Ulysses observations to further constrain shock inputs. We describe the results of that exercise, and show comparisons with Ulysses solar wind observations. The comparisons with the SWICS pickup proton density measurements at Ulysses and our model results are described in work by D. Intriligator. (Initial benchmarking of pickup proton modeling and Ulysses SWICS measurements: Comparisons with the three-dimensional MHD HHMS-PI simulation, submitted to Journal of Geophysical Research, 2010).

[8] We focus on the asymmetrical, 3-D, and time-dependent nature of the heliosphere, and we stress verification at each step, using quantitative comparisons of simulation results with spacecraft observations. Next we plan to use ACE, Ulysses, and Cassini observations to further constrain shock inputs, then extend the grid to 100 AU, and use those results to better understand Voyager 1 and Voyager 2 observations. Both Voyagers were still inside the TS when the Halloween 2003 shocks reached them, although the precise associations between the Halloween 2003 solar events and the arrival times of specific shocks in the plasma and field data from V2 and V1 have yet to be determined. We think, that by continuing to improve our model, and by using observations from ACE, Ulysses and Cassini to constrain shock inputs, that we can contribute toward determining those associations. We must also note that we would not necessarily expect our model runs to contain a TS, even though the locations where the TS was later observed by the Voyagers would be within the model grid. One reason is that we currently use a simple zero- to first-order extrapolation scheme to set our outer grid boundary condition, thus the model does not “feel” the full LISM pressure. We believe simulated conditions immediately upstream of the TS would be useful. Simulated conditions beyond the observed location of the TS, although incorrect, should still have some correlation with actual conditions.

[9] During the Halloween 2003 superstorm, three active regions (ARs) produced 124 soft X-ray flares, and more than 60 coronal mass ejections (CMEs) between 18 October and 5 November. Two CMEs hit Earth head-on resulting in huge geomagnetic storms. A review of the solar and terrestrial events was provided by Veselovsky et al. [2004]. A first set of predicted shock arrivals at Earth from some of these events was made as part of the Fearless Forecast [Dryer et al., 2004]; we refer to it again later.

[10] Although they were not based on a full 3-D MHD treatment, these earlier efforts to model the shock propagation did yield promising results. Because of the relative nearness of the Earth to the Sun, some of the specific nonlinearities and other effects that can only be accurately modeled in a full 3-D treatment did not overly influence the predictions. However, when modeling shock propagation to further distances, these effects can become large and thus must be included in a proper model. Furthermore, it should be emphasized that the unique orbits and positions of the various spacecraft and the spatially and temporally varying solar flares, CMEs, and high-speed streams necessitate full 3-D treatment. Finally, accurate and self-consistent input conditions at, or close to, the Sun are essential.

[11] This methodology, which includes accurate background and shock input descriptions along with full 3-D treatment, has been emphasized (as mentioned earlier) in exploratory work of Intriligator et al. [2005a, 2005b, 2005c, 2006, 2007, 2008], who initiated this 3-D MHD approach with the Hybrid Heliospheric Modeling System (HHMS) out to 5 AU without the inclusion of pickup protons. They also employed a computationally nonintensive “quick-look” 3-D kinematic model (Hakamada-Akasofu-Fry: HAFv.2). This latter model has also been used for real time space weather objectives [Fry et al., 2001, 2003; Dryer et al., 2004; McKenna-Lawlor et al., 2006; Smith et al., 2009b, 2009a].

[12] Section 2 will discuss the extension of HHMS to HHMS-PI to include consideration of pickup protons. Section 3 will lay out the sequence of simulation, verification, model, and shock input tuning steps performed. Section 4 gives results, and section 5 will contain discussion and concluding remarks.

2. The Model

[13] The Hybrid Heliospheric Modeling System (HHMS) began with an apparently simple idea for improving solar wind forecasts at Earth with a few days’ lead time [Detman et al., 2006]. A number of papers had already demonstrated predictive ability for solar wind at Earth using source surface models [Wang and Sheeley, 1988, 1990; Wang et al., 1996, 1997; Fry et al., 2001; Zhao and Hoeksema, 1993, 1994, 1995; Detman and Vassiliadis, 1997]. More recent results with source surface models are described by Arge and Pizzo [2000] and MacNiece [2009]. Yet these models are based on relatively simple physics (potential field extrapolation, via Laplace’s equation) from the photosphere through the solar corona to a specified “source surface” where an outer boundary condition of a purely radial magnetic field is applied. Source surface height is typically around 2.5$R_S$, where $R_S$ is the mean solar radius, 695000 km. The average Sun-Earth distance is about 215$R_S$, so these models typically
interface module generates time-dependent MHD boundary conditions for the solar wind model by interpolating between two SSCS maps separated in time by a solar rotation or less. This input path generates the slowly changing “background” solar wind. A more detailed discussion of the interface module is given later.

[16] The solar event input mode starts on the top right side of the block diagram in Figure 1. This input path applies an impulsive perturbation to the existing background boundary conditions in order to simulate the explosive release of energy in solar flares and CMEs. The intent of this input path is to introduce shock waves into the model grid, based on observed characteristics of type II radio sweeps and locations of solar flares and CMEs. The shock event inputs are start time, duration, latitude, longitude, perturbation radius (angle subtended from the center of the Sun), and shock speed. The preexisting boundary conditions are modified according to the Rankine-Hugoniot relations for the specified shock speed.

[17] The interface module does four things: (1) it translates from source surface map parameters to solar wind MHD parameters; (2) it extrapolates from source surface height to MHD boundary height (21.5 $R_S$ = 0.1 AU); (3) it introduces the effect of solar rotation; and (4) it introduces time dependence by interpolating in time between two source surface map files. The HHMS-PI interface module reads source surface maps in Flexible Image Transport System (FITS) format as generated and archived in near real time by NOAA’s Space Weather Prediction Center at http://www.swpc.noaa.gov/ws/. These maps are generated by the Wang-Sheeley-Arge Source Surface Current Sheet (SSCS) model [Arge and Pizzo, 2000] which is a potential field model with an added current sheet; in this model the source surface height is 2.5 $R_S$, but with the current sheet, the solution is given at 5$R_S$ These SSCS map files contain global maps, at 5$R_S$ and 5° × 5° angular resolution, of various parameters; we make use of the following three: radial magnetic field on the source surface, $ssBr$; flux tube expansion factor, $ssEf$; and foot point distance, on the photosphere, to the closest coronal hole boundary, $ssFd$. For efficiency in development and testing the HHMS-PI also has angular resolution of 5° × 5° to match the SSCS map files. In the radial direction the grid resolution is 1.76 $R_S$. We plan to improve grid resolution in future work.

[18] Pickup protons are insignificant at 0.1 AU, but for numerical reasons they cannot be set to zero or left uninitialized. Thus, they are initialized and held at very small values until the source terms in their conservation equations become significant. This occurs beyond 0.5 AU, for the small values we used in equations (9) and (10).

[19] HHMS-PI operates in Solar Equatorial spherical coordinates ($r$, $\theta$, $\phi$), and has ten MHD variables, as follows: three components of velocity ($U_r$, $U_\theta$, $U_\phi$), three components of magnetic field ($B_r$, $B_\theta$, $B_\phi$), and two densities and two pressures for solar wind and pickup protons, ($D_s$, $D_p$) and ($P_s$, $P_p$), respectively. The model grid covers 360° in longitude (the $\phi$ direction) with a periodic boundary condition; it goes from +57.5° to −57.5° in latitude (the $\theta$ direction), and 0.1 to 5.5 AU in radius. The computational MHD equations for these ten variables, in conservation form, are given in Appendix A. Note, by solving the MHD

covered less than 1.2% of that distance. The simple idea was that, by extrapolating a source surface solution only to 0.1 AU, it could be used to specify the lower boundary conditions of an MHD solar wind model (such as the present one and others), which would then cover the remaining 90% of the distance to Earth.

[14] A block diagram of HHMS-PI is shown in Figure 1. Note there are two independent paths by which solar observations drive the MHD boundary conditions.

[15] The background mode begins with solar magnetograms, top left in the block diagram. Daily magnetograms, over a solar rotation, about 27 days, are combined to make a global photospheric magnetic map. These photospheric maps provide the lower boundary condition for the WSA Source Surface Current Sheet model [Arge and Pizzo, 2000], which in turn gives a global solution for the magnetic field from the photosphere to the source surface. The HHMS-PI
[20] The MHD solar wind model in HHMS-PI operates under the assumption of hyperbolic boundary conditions. This means the flow speed on the grid boundary must be faster than any characteristic wave speed in the plasma. Specifically, this means, \( U_r > \gamma B_s \), where \( B_s \) is the fast mode wave speed and \( F_s = C_s^2 + V_A^2 \), where \( C_s \) is the sound speed, and \( V_A \) is the Alfvén speed; \( C_s = \gamma P_s / D_s \), and \( V_A^2 = B^2 / (\mu D_s) \). Two difficulties are encountered in designing the interface. One difficulty is that the interface model has to mimic the main plasma physics of the corona that is missing from all source surface models, and that is computationally intensive for MHD models. The second difficulty is that our original choice of 0.1 AU for the lower grid boundary has turned out to be too close to the Sun (closer than the Alfvén critical point) a little too often. The first problem is fundamental. Our approach to solve it has been to develop a set of empirical formulas, containing adjustable parameters, for converting three SS map parameters into eight MHD parameters. Due in part to its empirical character, our interface module keeps evolving as we continue to learn and test (benchmark) new approaches. We will say more about this in section 4. The second problem is not fundamental; we can simply raise the lower grid boundary. This would reduce, but not eliminate, the occurrence of solar wind conditions when the Alfvén critical point is within the grid. This would also increase the volume of space that this simple empirical model must account for.

[21] The empirical translation from three source surface parameters to eight MHD boundary condition parameters currently contains five free “tuning” parameters that we tune (optimize) for agreement of the model output with spacecraft observations during quiet (background) solar wind conditions. This could be viewed as a five dimensional nonlinear optimization problem, but, by using observable flow invariants such as \( r^2 B_r \) and \( r^2 D_s U_r \) it effectively reduces to a three dimensional search; also the optimum turns out to be smooth and broad. This allows us to find an adequate near-optimum tuning with a reasonable number of model runs.

[22] The choice of a function to maximize, by tuning, is also important. In tuning for agreement with ACE solar wind observations, we used the mean of five skill scores for five different solar wind quantities: speed, \( U_r \); number density, \( N_s \); mass flux, \( FM = D_s U_r \); and \( (B_r - B_\alpha) \). Note, \( (B_r - B_\alpha) \) is the projection of the field onto the Parker spiral; we use it as a measure of interplanetary magnetic field (IMF) polarity. Skill score, also known as prediction efficiency, is defined as 1.0 minus the ratio of mean squared error \( (MSE) \) to the sample variance \( (VAR) \):

\[
\text{skill} = PE = 1 - \frac{MSE}{VAR},
\]

where \( MSE = \frac{1}{N} \sum_{i=1}^{N} (f_i - x_i)^2 \) and \( VAR = \frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})^2 \). In section 4, we will give details of our selection of tuning criteria and show some results in section 5.

However, because the correlation coefficient is a commonly used and familiar parameter, we show both the skill and correlation coefficient on our plots. The correlation coefficient \( r_c \) is given by

\[
r_c = \frac{\sum (f_i - \bar{f})(x_i - \bar{x})}{\sqrt{\sum (f_i - \bar{f})^2 \sum (x_i - \bar{x})^2}}.
\]
and \( W \times \delta V = V_{\text{exp}} \delta V_f \) is the polytropic index for solar wind; \( B_{\text{spec}} \), a fixed strength for the magnitude of the radial magnetic field; here \( B_{\text{spec}} \) is the median of \( \text{ssBr} \) for an individual SS map; and \( \gamma \) is the polytropic index for solar wind protons. As explained by Detman et al. [2006], the source surface field, \( \text{ssBr} \), fluctuates from map to map. In our interface module these fluctuations must be removed to prevent introduction of magnetic monopoles into the model grid. Equation (4) does this by replacing the fluctuating \( \text{ssBr} \) with \( B_{\text{spec}} \).

For the results presented here, our interface module used the following formulas to translate and extrapolate from SS map parameters at 21.5 Rs (0.1 AU):

\[
U_r = V_{\text{min}} + \text{delV/} \text{ssBr} \text{exp} + 7.4 \left( \text{ssF}/\text{ssBr} \text{exp}^2 - 3.5 \right),
\]

(1)

\[
U_\phi = 0,
\]

(2)

\[
U_\phi = \Omega R_\phi \sin \theta,
\]

(3)

\[
B_r = B_{\text{spec}} \text{ssBr} / B_{\text{median}},
\]

(4)

\[
B_\theta = 0,
\]

(5)

\[
B_\phi = V_\phi B_r / U_r,
\]

(6)

where \( V_\phi = U_\phi - \Omega r \sin \theta \),

\[
D_s = (B_{\text{spec}} M_A / U_r)^2 / \mu_0,
\]

(7)

\[
P_s = (D_s / \gamma)(U_r / M_A)^2,
\]

(8)

\[
D_p = 10^{-20},
\]

(9)

\[
P_p = 10^{-14}.
\]

(10)

Table 2. Shock Inputs Adjusted to Match ACE Observed Shock Arrivals

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<th>FF Event Number</th>
<th>DOY</th>
<th>VS.g</th>
<th>TAU (h)</th>
<th>LAT</th>
<th>LON</th>
<th>TOAOA</th>
<th>TTO (h)</th>
<th>TOAAS</th>
<th>TTS (h)</th>
<th>VS.h</th>
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<td>-56</td>
<td>294.819</td>
<td>50.832</td>
<td>294.704</td>
<td>48.07</td>
<td>575.0</td>
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</table>

*FF, Fearless Forecast event number, as in Table 1; DOY, day of year with fraction translated from Table 1, second and third columns; VS.g, adjusted shock speed on iteration “g”; TAU, shock driving time duration in hours with fraction; LAT, flare heliolatitude (same as in Table 1); LON, flare heliolongitude; TOAAO, time of shock ACE arrival observed (blank means no observed shock at ACE could be paired with this solar event); TTO, shock travel time observed (column 7 – column 2) × 24; TOAAS, time of shock ACE arrival simulated; TTS, shock travel time simulated; VS.h, new adjusted shock speed for iteration “g” (VS.h = TTS/TTO × VS.g, as explained in text).
with the specified constant $B_{SPEC}$. For our simulation of the Halloween 2003 events, we used the first 200 days of 2003 for background mode tuning, and we arrived at the following parameter values:

$$V_{min} = 154 \text{ (km/s)},$$

$$delV = 300 \text{ (km/s)},$$

$$V_{esp} = 0.3,$$

$$M_s = 1.28,$$

$$M_A = 1.00.$$

[26] We set the polytropic index, $\gamma = 1.5$ based on work by Totten et al. [1996]. We use $B_{SPEC} = 500nT$; this value gives average field strengths at Earth that are usually slightly weaker than observed, however it allows us to keep the Alfvén Mach number tuning parameter, $M_A \geq 1.00$, consistent with our assumption of hyperbolic boundary conditions.

[27] As a starting point we adopted the stationary, spherically symmetrical neutral hydrogen distribution of Wang et al. [2000], see Appendix A. In future work, we plan to implement a more realistic neutral hydrogen model that has uniform speed, direction, upstream density, and includes conservation of mass for the neutral hydrogen within the model grid. This might be accomplished with a relatively simple model for the neutral hydrogen, however the HHMS-PI model will then need to be modified to operate in Solar Ecliptic (inertial) coordinates.

3. The Method

[28] Our approach is incremental. We created the HHMS-PI code by modifying its predecessor, HHMS, to solve the equations of ideal MHD solar wind with pickup protons, as described in Appendix A. Next, we used the first 200 days of 2003 for background mode tuning.

[29] Next we introduced the Halloween 2003 series of solar events. We started with the shock strengths, locations, times, and durations given in Table 1. In Table 1, the first seven columns are the Fearless Forecast (FF) event number, the date, time, heliolatitude, heliolongitude, shock speed, and duration given in hhmm format. (The remaining five columns are not used by HHMS-PI.) These parameters were originally posted to an e-mail list in near real time, following solar events, as the Fearless Forecast [Dryer et al., 2004]. These values were used in HHMS-PI to apply shock perturbations directly to the background mode boundary conditions. We simulated the interval from day 285 of 2003 through the end of the year. After applying the shock perturbations, we again compared HHMS-PI results with ACE observation for this time period. Not surprisingly, the agreements between simulated and observed shock arrivals at ACE were less than perfect. In fact, inspection of time series alone was not sufficient to deduce many of the associations between input shock perturbations and simulated (or observed) shock arrivals at ACE.

[30] To make this association, we made radius-time (r-t) plots of an especially designed shock index, $d/dr \log(r^4 \rho F_S)$, along the Sun-Earth line, where $\rho = D_s + D_p$ is total mass density, and, $F_S$ is the fast mode wave speed, $F_S^2 = \gamma P_T/\rho + B^2/(\mu_0 \rho)$, where $P_T = P_s + P_p$ is the total thermal pressure. Figure 2 shows such an r-t plot along the Sun-Earth line from a model run of the Halloween 2003 events. With the associations in hand, we then used the simulated time series at ACE, to “zoom in” and get more accurate simulated shock arrival times at ACE.

[31] We then used the ratios of simulated to observed shock travel times to adjust the shock speed inputs in an iterative tuning process. For an isolated shock event this adjustment process usually converges in three or four iterations to make the simulated shock arrival time closely match the observed. For the rapid fire solar events of Halloween 2003, pairing FF events at the Sun with observed shocks at ACE is challenging; shock interactions complicated both the tuning and matching processes. We consider our current pairings, shown in Table 2, to be preliminary. Table 2 shows one iteration (g to h) of the shock speed adjustment process. In Table 2, date and time have been converted to fractional day of year; TOAAO is time of arrival, ACE, observed; TTO is travel time, observed, in hours; TTS is travel time simulated; and VS.h is the new adjusted shock speed, $VS.h = VS.g \cdot TTS/TTO$. Figure 3 shows the resulting time series comparisons of HHMS-PI with ACE for the Halloween 2003 interval.

[32] Next, we extended the model grid to 5.5 AU, keeping the neutral hydrogen density at $\infty$, $N_\infty = 0.1 \text{ cm}^{-3}$, repeated the last run (that is, we use the ACE tuned shock inputs), and compared model results with observations at Ulysses. Again, this first comparison was not impressive. In order to obtain good comparisons at both ACE and Ulysses, we undertook a somewhat trial and error bituning exercise; adjusting mainly the heliolatitude (LON), disturbance radius (RAD), and shock speed (VSH). Table 3 gives the results of that exercise. Figure 4 is an r-t plot, like Figure 2, but showing shocks’ propagation along the Sun-Ulysses line, and Figure 5 compares the HHMS-PI simulated time series with Ulysses solar wind observations at 5.25 AU and 103 degrees west of Earth in heliolongitude.

[33] Finally, we repeated this last run with the neutral hydrogen density set to zero in order to isolate the effect of pickup protons on shock propagation. The results of that exercise are shown in Table 4, as promised by the title of this paper. (At ACE, we found no differences in simulated shock arrival times.) In Table 4, $DNH_\infty = N_\infty m_p$ is the mass density of neutral hydrogen at infinity (see Appendix A), and DIFF is the delay in shock arrival, in days, due to pickup ions. Our results, in Table 4, show unambiguously that solar-generated interplanetary shock wave speeds are reduced by the presence of pickup protons from the LISM neutral hydrogen flowing into the heliosphere.

4. Discussion

[34] A notable aspect of the shock input bituning (to match shock arrivals at both ACE and Ulysses) is that we could not reproduce the high solar wind speeds seen at Ulysses around day 320 using only the original Fearless Forecast events. Meanwhile, de Koning et al. [2005] indicated the occurrence of an unusually fast CME originating from beyond the visible disk of the Sun on 7 November at 1554 UT. On the basis of that information, we added the event listed as FF 520.2 in the first column of Table 3. A longitude of W120, and latitude of S18 is consistent with this event coming from the same active region (NOAA/
Figure 3. Comparison of HHMS-PI simulated time series at Earth with ACE solar wind observations for the Halloween 2003 study interval. Blue is ACE data. Red is HHMS-PI. Magenta (top only) is the HHMS-PI boundary condition at the sub-Earth point.
Table 3. Shock Inputs Adjusted to Match Both ACE and Ulysses

<table>
<thead>
<tr>
<th>Event Date</th>
<th>Event Time</th>
<th>DOY</th>
<th>LAT (deg)</th>
<th>LON (deg)</th>
<th>RAD (deg)</th>
<th>VSH (km/s)</th>
<th>TAU (h)</th>
<th>FF</th>
</tr>
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<tr>
<td>19 Oct 2003</td>
<td>1650</td>
<td>292.701</td>
<td>5</td>
<td>-56</td>
<td>102</td>
<td>519.6</td>
<td>1.3</td>
<td>507</td>
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<td>21 Oct 2003</td>
<td>0347</td>
<td>294.158</td>
<td>10</td>
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<td>100</td>
<td>517.0</td>
<td>0.7</td>
<td>508</td>
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<tr>
<td>22 Oct 2003</td>
<td>0938</td>
<td>295.401</td>
<td>-2</td>
<td>-22</td>
<td>100</td>
<td>781.5</td>
<td>3</td>
<td>509</td>
</tr>
<tr>
<td>23 Oct 2003</td>
<td>0827</td>
<td>296.352</td>
<td>-21</td>
<td>-88</td>
<td>108</td>
<td>1276.0</td>
<td>1.5</td>
<td>510</td>
</tr>
<tr>
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<td>298.177</td>
<td>-15</td>
<td>-43</td>
<td>120</td>
<td>530.0</td>
<td>2</td>
<td>511</td>
</tr>
<tr>
<td>26 Oct 2003</td>
<td>0617</td>
<td>299.262</td>
<td>-18</td>
<td>-43</td>
<td>120</td>
<td>574.1</td>
<td>3</td>
<td>512</td>
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<tr>
<td>26 Oct 2003</td>
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<td>299.733</td>
<td>5</td>
<td>32.6</td>
<td>70.2</td>
<td>1027.0</td>
<td>3.5</td>
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<tr>
<td>28 Oct 2003</td>
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<td>301.460</td>
<td>-16</td>
<td>-8</td>
<td>120</td>
<td>1951.0</td>
<td>3</td>
<td>514</td>
</tr>
<tr>
<td>29 Oct 2003</td>
<td>2044</td>
<td>302.864</td>
<td>-14</td>
<td>1</td>
<td>123</td>
<td>1612.4</td>
<td>1.5</td>
<td>515</td>
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<tr>
<td>1 Nov 2003</td>
<td>2234</td>
<td>305.940</td>
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<td>61</td>
<td>120</td>
<td>820.9</td>
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<td>2 Nov 2003</td>
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<td>-14</td>
<td>82.53</td>
<td>158</td>
<td>1791.4</td>
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<td>517</td>
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<tr>
<td>3 Nov 2003</td>
<td>0124</td>
<td>307.058</td>
<td>10</td>
<td>85</td>
<td>100</td>
<td>725.0</td>
<td>1.8</td>
<td>518</td>
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<tr>
<td>3 Nov 2003</td>
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<td>307.414</td>
<td>8</td>
<td>77</td>
<td>120</td>
<td>1131.3</td>
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<td>519</td>
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<tr>
<td>4 Nov 2003</td>
<td>1943</td>
<td>308.822</td>
<td>-19</td>
<td>78.84</td>
<td>102</td>
<td>1580.7</td>
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<td>311.663</td>
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<td>120</td>
<td>100</td>
<td>1682.7</td>
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<td>520</td>
</tr>
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<td>1335</td>
<td>315.566</td>
<td>-3</td>
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<td>93.7</td>
<td>807.0</td>
<td>3</td>
<td>521</td>
</tr>
<tr>
<td>13 Nov 2003</td>
<td>0924</td>
<td>317.392</td>
<td>1</td>
<td>-90</td>
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<td>100</td>
<td>547.0</td>
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<td>523</td>
</tr>
<tr>
<td>18 Nov 2003</td>
<td>0747</td>
<td>322.324</td>
<td>0</td>
<td>-18</td>
<td>221.1</td>
<td>918.4</td>
<td>3</td>
<td>524</td>
</tr>
<tr>
<td>20 Nov 2003</td>
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<td>324.324</td>
<td>1</td>
<td>14</td>
<td>104.9</td>
<td>997.9</td>
<td>0.8</td>
<td>525</td>
</tr>
</tbody>
</table>

*DOY, date and time translated to day of year 2003 with fraction; LAT, shock input heliolatitude; LON, shock input heliolongitude; RAD, shock input radius; VSH, shock input speed; TAU, shock input duration; FF, event sequence number.

SWPC AR 10486) that produced FF520, FF517, and/or FF514. When we added this event to our shock inputs and adjusted the shock speed to make the simulated shock arrive at day 318.984, we got a significantly better match to Ulysses velocities around that time, but we also got a greatly improved match with a reverse shock at Ulysses near day 320, that produced the highest speeds at Ulysses in the study interval.

Even in its simplest form that ignores practically all microphysics, ideal MHD can often produce useful global-scale results simply because it conserves mass, momentum, and energy. On the other hand, it is possible to modify or extend the equations of ideal MHD to include specific effects that arise from a more detailed consideration of the physics. The work described here is an example of this. By adding just the most basic physics of pickup ions to our model, we have brought it into better agreement with spacecraft observations. In extending our model to 100 AU, we expect that in order to reproduce temperature vs. distance and other observations in the more distant outer heliosphere, we will find it helpful to add more such modifications. In particular, our current use of a polytropic index to implicitly represent thermal heat conduction based on work by Totten et al. [1996] is certainly not valid far beyond 1 AU; we plan to rectify this by introducing some explicit form of heat or energy transport, such as the collisionless electron heat conduction of Hollweg [1976], or the Alfvén wave energy flux of Usmanov et al. [2000]. Also since energetic particles (pickup ions) account for most of the thermal pressure in the distant heliosphere, we may eventually want to consider the effect of turbulence energy resulting from the effect of the pickup process on the magnetic field, as described by Isenberg et al. [2010].

Large-scale models, such as HHMS-PI, generally cannot include microscale physics in detail, even when it is well known. Consequently, the success of a large-scale model often depends on finding useful (or even correct) empirical relationships that capture the emergent macroscale consequences of the microphysics. The interface module in HHMS-PI takes this approach. It maps source surface model outputs at 5Re into MHD boundary conditions at 21.5RS using a set of empirical formulas (equations (1)–(8)) to produce the background solar wind in HHMS-PI. Comparison of equations (1)–(8) here with the corresponding equations of Detman et al. [2006] show that the interface module has evolved. In fact, at this stage of development, the interface model continues to evolve, as our understanding of the corona improves. In the near future we hope to explore other important parts of the model for further improvement, such as our current 5° × 5° angular grid resolution, our oversimplified background neutral hydrogen distribution, or our diffusive, modified two-step Lax-Wendroff numerical scheme [Han et al., 1988]. In spite of these self-deprecating statements, we have prominently displayed skill scores, and correlation coefficients, on all

Figure 4. Sun–Ulysses r-t plot of shock index. Circles mark observed shock arrivals; plus signs mark simulated shock arrivals. Dotted lines mark magnetic sector boundaries.
Figure 5. Comparison of HHMS-PI simulated time series at Ulysses with Ulysses solar wind observations for the Halloween 2003 study interval. Blue is Ulysses SWOOPS data. Red is HHMS-PI.
Table 4. Shock Arrival Delays at Ulysses Due to Pickup Protons

<table>
<thead>
<tr>
<th>FF</th>
<th>DOYSUN</th>
<th>OBSULY</th>
<th>DNH0 = 0.1</th>
<th>DNH0 = 0</th>
<th>DIFF (days)</th>
</tr>
</thead>
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<tr>
<td>514</td>
<td>301.460</td>
<td>311.801</td>
<td>312.632</td>
<td>311.877</td>
<td>0.755</td>
</tr>
<tr>
<td>517</td>
<td>306.718</td>
<td>316.884</td>
<td>317.876</td>
<td>317.000</td>
<td>0.876</td>
</tr>
<tr>
<td>520</td>
<td>308.822</td>
<td>317.641</td>
<td>318.194</td>
<td>317.491</td>
<td>0.703</td>
</tr>
<tr>
<td>520.2</td>
<td>311.664</td>
<td>319.000</td>
<td>319.167</td>
<td>318.600</td>
<td>0.567</td>
</tr>
<tr>
<td>521</td>
<td>315.566</td>
<td>326.851</td>
<td>327.004</td>
<td>326.105</td>
<td>0.899</td>
</tr>
<tr>
<td>522</td>
<td>322.324</td>
<td>333.810</td>
<td>335.145</td>
<td>334.534</td>
<td>0.611</td>
</tr>
</tbody>
</table>

*FF, event sequence number; DOYSUN, FF solar event day of 2003 with fraction; OBSULY, observed shock arrival at Ulysses day of 2003 with fraction; DNH0.1, simulated Ulysses shock arrival day of 2003 with fraction for the case of neutral hydrogen density at \( \omega = 0.1 \) cm\(^{-3}\); DNH0.0, simulated Ulysses shock arrival day of 2003 with fraction for the case of neutral hydrogen density equal to zero; DIFF, \( \text{DIFF} = \text{DNH0.1} - \text{DNH0.0} \).*

5. Conclusions

[37] The general agreement of HHMS-PI simulation results with ACE observations shown in Figure 3, and with Ulysses observations shown in Figure 5, demonstrate that HHMS-PI is a suitable foundation for extending our benchmarking process for tracking shocks out to Cassini and beyond. Our results also clearly demonstrate the impact of including pickup proton effects in our model. This important success highlights the fact that our full 3-D model offers extensibility to include a range of physical phenomena that can even further strengthen our model. We are very encouraged by the level of agreement shown here, and we plan to continue addressing the bountiful avenues of model applications and improvements that we have identified.

Appendix A

[38] HHMS-PI computational equations (heliocentric spherical coordinates):

\[
\begin{align*}
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial \mathbf{G}}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial \mathbf{H}}{\partial \phi} &= \mathbf{S},
\end{align*}
\]

where

\[
\mathbf{U} = \begin{pmatrix}
\mathbf{U}_r \\
\mathbf{U}_\theta \\
\mathbf{U}_\phi \\
\mathbf{U}_r \\
\mathbf{U}_\theta \\
\mathbf{U}_\phi
\end{pmatrix},
\]

\[
\mathbf{F} = \begin{pmatrix}
r^2 \rho \mathbf{U}_r \\
r^3 \rho \left( \mathbf{U}_\theta^2 + \frac{\rho}{(\gamma - 1) \rho} + \frac{2}{r^2} - A_r^2 \right) \\
r^3 \rho \mathbf{U}_\theta \\
r^3 \rho \mathbf{U}_\phi \\
r^3 \rho \mathbf{U}_r \\
r^3 \rho \mathbf{U}_\phi
\end{pmatrix},
\]

\[
\mathbf{G} = \begin{pmatrix}
0 \\
0 \\
r^2 \rho \sin \theta \mathbf{U}_\theta \\
0 \\
r^2 \rho \sin \theta \mathbf{U}_\phi \\
r^2 \rho \sin \theta \mathbf{U}_r
\end{pmatrix},
\]

\[
\mathbf{H} = \begin{pmatrix}
0 \\
0 \\
r^2 \rho \mathbf{V}_\phi \\
r^2 \rho \mathbf{V}_\theta \\
r^2 \rho \mathbf{V}_r
\end{pmatrix},
\]

\[
\mathbf{S} = \begin{pmatrix}
-\mathbf{q}_e \\
r_p \left( \mathbf{U}_\theta^2 + \mathbf{U}_\phi^2 + \frac{2}{r^2} + A_r^2 \right) - \rho GM_S - r^2 \mathbf{U}_qex \\
r_p \left( -r^2 \mathbf{U}_\theta \mathbf{U}_\phi \mathbf{U}_r \mathbf{U}_\theta - \mathbf{A}_r \mathbf{A}_\theta \mathbf{U}_r \mathbf{U}_\theta \right) - \mathbf{q}_e \mathbf{V}_ex \\
r_p \left( -r^2 \mathbf{U}_\theta \mathbf{U}_r \mathbf{U}_\phi \mathbf{U}_r \mathbf{U}_\theta - \mathbf{A}_r \mathbf{A}_\theta \mathbf{U}_r \mathbf{U}_\theta \right) - \mathbf{q}_e \mathbf{V}_ex \\
0 \\
0 \\
r^2 \mathbf{U}_\theta \mathbf{U}_\phi \mathbf{U}_r \mathbf{U}_\theta \mathbf{U}_\phi \mathbf{U}_r \mathbf{U}_\theta
\end{pmatrix},
\]

where \( \rho = \rho_r + \rho_p, \mathbf{P} = \mathbf{P}_L + \mathbf{P}_P, \mathbf{P}_S = 2 \rho_s \mathbf{R}_S, \mathbf{P}_I = \rho \mathbf{R}_I, \mathbf{U}_r = \mathbf{U}_r^2 + \mathbf{U}_\theta^2 + \mathbf{U}_\phi^2, \mathbf{A}_r^2 = \mathbf{A}_r^2 + \mathbf{A}_\theta^2 + \mathbf{A}_\phi^2, \mathbf{B}_r, \mathbf{B}_\theta, \mathbf{B}_\phi = \mathbf{B}_r, \mathbf{B}_\theta, \mathbf{B}_\phi \). Here \( \mathbf{U} \) denotes velocity in the inertial frame, \( V \) denotes...
velocity in the solar corotating frame, \( \mathbf{U} = \mathbf{V} + \mathbf{w} \), where \( \mathbf{w} = \Omega \times \mathbf{r} = \Omega r \sin \theta \phi \), and \( \Omega \) is the solar rotation rate.

[39] Also, \( \rho_s \) and \( \rho_p \) are solar wind density and pressure; \( \rho_s \) and \( \rho_p \) are pickup ion density and pressure. The ratio of specific heats for pickup ions is taken to be 5/3; the polytropic index for the solar wind is \( \gamma = 1.5 \). For our steady state model, used only to initialize our time-dependent model, and for this initial development of the time-dependent model, we use the spherically symmetric and stationary (with respect to the Sun) neutral hydrogen distribution given by Wang et al. [2000]: \( N_H = N_0 e^{-\lambda r} \), where \( N_0 = 0.1 \) cm \(^{-3} \), and \( \lambda = 4 \) AU. Following Whang [1998] and Usmanov and Goldstein [2006], the production rates for interstellar pickup ions are given by: \( q_{ex} = \epsilon_m N_S N_H U_1 \), \( q_{ph} = \epsilon_m N_H \left( \frac{2}{\sigma} \right) \), with \( \sigma = 2 \times 10^{-15} \) cm\(^2\), and \( \nu = 9 \times 10^{-8} \) s\(^{-1}\), as in work by Usmanov and Goldstein [2006]. We plan to introduce more realistic models for \( N_H \) in future work. Also, for some runs in the current work, we set \( N_H = 0 \) to determine the specific affects due to pickup protons.

[40] Acknowledgments. We thank the NOAA Space Weather Prediction Center for generating and maintaining the archives of WSA source surface maps and making them available. We thank the ACE and Ulysses teams and the NSSDC for the IMF, plasma, and plasma wave data and trajectory information. We thank A. Usmanov for invaluable help in deriving the computational equations in Appendix A. This work was supported in part by NASA grant NNX08AE40G with Carmel Research Center and in part by Carmel Research Center. T. R. Detman thanks the Ubuntu, Octave, OpenOffice.org, and LaTeX open source project communities.

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References


