Modeling Secondary Neutral Helium in the Heliosphere

Hans-Reinhard Müller, Eberhard Möbius and Brian E. Wood

1 Department of Physics and Astronomy, Dartmouth College, Hanover, NH 03755, USA
2 Center for Space Plasma and Aeronomic Research, University of Alabama, Huntsville, AL 35805, USA
3 Space Science Center and Department of Physics, University of New Hampshire, Durham, NH 03824, USA
4 Naval Research Laboratory, Space Science Division, Washington, DC 20375, USA

E-mail: hans.mueller@dartmouth.edu

Abstract. An accurate, analytic heliospheric neutral test-particle code for helium atoms from the interstellar medium (ISM) is coupled to global heliospheric models dominated by hydrogen and protons from the solar wind and the ISM. This coupling enables the forward-calculation of secondary helium neutrals from first principles. Secondaries are produced predominantly in the outer heliosheath, upwind of the heliopause, by charge exchange of helium ions with neutral atoms. The forward model integrates the secondary production terms along neutral trajectories and calculates the combined neutral helium phase space density in the innermost heliosphere where it can be related to in-situ observations. The phase space density of the secondary component is lower than that of primary neutral helium, but its presence can change the analysis of primaries and the ISM, and can yield valuable insight into the characteristics of the plasma in the outer heliosheath.

1. Introduction

The detection of neutral interstellar helium atoms close to Earth has enabled a detailed characterization of key parameters of the local interstellar medium (LISM), including densities, velocity magnitude and direction, and LISM temperature. The LISM is the portion of the interstellar medium with which the Sun and its solar wind interacts, and it is thought to be a representative sample of the so-called Local Interstellar Cloud, the interstellar cloud that the heliosphere currently traverses on its galactic orbit.

The preference on studying helium as a key heliospheric neutral particle species is owed to helium being the species that suffers the least changes (losses, processing) on its way from the LISM to the detectors in the inner solar system, while having a high abundance in the ISM as compared to heavier elements. There are several ways to detect neutral helium atoms of interstellar origin in the innermost heliosphere, and this paper focuses on the direct detection through instruments on board of the Ulysses and IBEX missions. Both missions have a high sensitivity to helium, very good directional accuracy, and good energy resolution. The helium fluxes measured at the spacecraft hence can be related well to the neutral helium velocity distribution function (VDF) in the inner heliosphere.
With the help of archival \textit{Ulysses} data and data collected by \textit{IBEX} since 2009, it was possible to constrain the LISM parameters through the analysis of primary interstellar helium whose source is the LISM itself (Bzowski et al. 2015, Möbius et al. 2015, Wood, Müller & Witte 2015, McComas et al. 2015). A secondary component of neutral helium was noticed as well, albeit at a lower flux level. Efforts have been undertaken to separate the primary and the secondary signal from each other (Kubiak et al. 2014, 2016). One of the aims of such studies is to shore up the accuracy of the determination of primary neutral helium (and hence the pristine LISM itself) even further than with the prior analyses where the perturbation of the primaries due to the presence of secondaries was neglected.

Another, even stronger motivation for investigating the secondary helium component is rooted in the physics of their creation: Secondary helium is born predominantly through charge exchange in the outer heliosheath between the interstellar bow shock and the heliopause. The charge exchange collision converts a shock-decelerated, singly ionized He$^+$ ion into a secondary neutral helium atom, while maintaining the original momentum of the parent ion; the neutral can be detected by \textit{Ulysses} and \textit{IBEX} just like any other neutral helium atom. Secondaries therefore open a very intriguing window of remote sensing of the plasma conditions in the outer heliosheath, including the ion velocity distribution, using neutral detectors as telescopes taking advantage of this window. Thus far only \textit{Voyager 1} has pushed into the outer heliosheath and is taking measurements very close to the heliopause. Both \textit{Voyager} 1 and 2, when it crosses the heliopause, have limited instrumental capabilities to diagnose the outer heliosheath ion population and can provide only local samples, while, through secondary neutrals, \textit{IBEX} provides an image over a large portion of the sky.

### 2. Framework of Determining Secondary Helium

#### 2.1. Physics Context

Through an assessment of cross sections and the characteristic parameters of collision partners, three channels of charge exchange (c.x.) have been identified as the most important ones for the creation of secondary helium in the heliosphere (Bzowski et al. 2012):

- \textbf{He}+\textbf{He}^+ \rightarrow \textbf{He}^++\textbf{He} — simple helium c.x. between primary neutral helium and helium ions; dominant in the outer heliosheath where both particle species are abundant; particularly He ions in the LISM have densities comparable to those of neutral He (Slavin & Frisch 2008).

- \textbf{He}+\textbf{He}^{++} \rightarrow \textbf{He}^{++}+\textbf{He} — double c.x. which has a large cross section; dominant in the solar wind where there are plenty of \textit{α} particles, with a $1/r^2$ falloff; very little \textit{α} in the LISM.

- \textbf{He}^++\textbf{H} \rightarrow \textbf{He}+\textbf{p} — c.x. with neutral hydrogen; the cross section is low, but there is a higher density of neutral H partners than He, especially in the hydrogen wall that is co-located with the outer heliosheath.

The third reaction turns out to be much less important than the first one (Bzowski et al. 2012), and the second one is not relevant for spacecraft in the inner solar system, such as \textit{Ulysses} and \textit{IBEX}, which avoid pointing their detectors sunward, i.e. the expected arrival direction of these particular secondaries (neutralized solar wind).

Focusing on the dominant c.x. interaction He+He$^+ \rightarrow$ He$^+$+He, it is a generally valid assumption that the newly born neutral bears the velocity characteristics of the former He$^+$ ion. In the outer heliosheath this means that the secondaries are slower and correspond to a higher temperature, than the primaries because they originate from heated and decelerated ions. The lower velocity translates to stronger gravitational deflection for secondaries that reach the innermost heliosphere, and to a lower energy than the primaries, making them potentially harder to detect.

For simplicity, different ion species in interstellar plasma and solar wind plasma are assumed to be in equilibrium so that the velocity state of a He$^+$ ion is estimated with the help of the general plasma state, the latter being dominated by protons. The velocity state of the primary
neutral helium can be estimated from prior test-particle simulations of this species (Müller 2012; Müller & Cohen 2012; Müller et al. 2013), and for the remote distances of the outer heliosheath, the primary helium can at first be well approximated by a shifted Maxwellian.

Once a secondary helium atom has been created through c.x., it is transported forward in a test-particle code (section 2.2 below) that has been developed for the accurate calculation of primary He in the heliosphere. Before reaching the detector, secondaries and primaries alike are subjected to the same types of losses on their trajectory from their source to the detector. In contrast to primary He with their “point source at infinity”, the secondaries have distributed, non-zero production terms along the entire Keplerian trajectory that need to be integrated to get the right flux at a point of interest like the spacecraft detector. Production and losses together give a net phase space density at the velocity that this trajectory corresponds to at the detector. Repeating the procedure for all different arrival directions, and different possible velocity magnitudes, is equivalent to testing a whole variety of trajectories that all intersect at the detector, each single one with integrated production and loss terms. This characterizes an entire velocity distribution function (VDF) of secondaries at the location of the spacecraft which can be converted into predicted fluxes. This method of calculating the secondary VDF operates from first principles and makes no assumptions about the shape of the VDF at any reference distance. As creation and loss calculations depend on the global heliosphere background model, the results for secondaries will depend on the background heliosphere model sensitively, more so than the primary He calculations. The secondary results, just like the primary ones, also depend on the accuracy of our knowledge of the c.x. cross sections, and on the underlying assumptions listed above, including the assumptions about the VDF (both neutral and ionized) in the pristine LISM being Maxwellian, and the plasma components being in equilibrium.

2.2. Calculation Method

2.2.1. Dartmouth test-particle forward modeling. The Dartmouth test-particle code and its results when applied to primary helium have been described elsewhere (Müller 2012; Müller & Cohen 2012; Müller et al. 2013; Wood & Müller 2015; Wood et al. 2015). In summary, the calculation method is an ab-initio modeling that assumes a fixed neutral helium VDF in the undisturbed LISM and transports neutral particles from a distant reference distance to the location of spacecraft such as Ulysses and IBEX. For each particle, quantities that are conserved along the entire trajectory (total energy, angular momentum, and eccentricity vector; Müller & Cohen (2012)), are used to determine in one algebraic step the neutral He velocity at a desired point in space, when the velocity in the pristine LISM (“at infinity”) is given. During transport to the position of the spacecraft, the distribution will be primarily affected by Sun’s gravity, and through photoionization by solar EUV photons. Moreover, c.x. losses and those by electron impact ionization contribute changes. The latter two loss channels require the knowledge of the global plasma heliosphere background model which is obtained from an MHD model independent from the neutral He atoms (e.g., Müller et al. 2008); in this way the test-particle code is coupled to the global heliosphere model. The repetition of the trajectory method for all trajectories that intersect at the desired point of interest yields a complete primary neutral He VDF at that point. Sample figures of these primary VDFs are shown in the references cited above.

For exploration purposes, an axisymmetric global heliosphere model is chosen as background model here, to begin with the simplest possibility. A heliocentric Cartesian coordinate system is defined, with the $x$ axis antiparallel to the LISM flow, and $y$ and $z$ perpendicular coordinates. The parameters characterizing interstellar matter and the solar wind are given in Table 1; they are just an example setup (proof of concept), without the claim of being the most appropriate or realistic parameters. The parameters correspond to a two-shock heliosphere with a weak interstellar bow shock present, hence in what follows, we make reference to a bow shock even though the presence of such a shock is not universally accepted.
Table 1. Parameters, both for LISM and the solar wind, of the global heliosphere background model and the neutral test-particle code. Units for speed, temperature $T$, and number densities $n$ are km/s, K, and cm$^{-3}$, respectively. Symbols p, H, and He signify protons, hydrogen, and helium, the latter in various charge states. The $\text{He}^{++}/p$ and $\text{He}^+/p$ columns represent plasma abundance ratios.

|       | speed | $T$  | $n_p$ | $\text{He}^{++}/p$ | $\text{He}^+/p$ | $n_H$ | $n_{He}$ |
|-------|-------|------|-------|---------------------|------------------|-------|---------|
| LISM  | 26.3  | 7000 | 0.047 | 0.0079              | 0.36             | 0.216 | 0.018   |
| SW at 1 AU | 400  | $10^5$ | 5.0   | 0.04                | 0.001            | -     | -       |

2.2.2. Secondary helium modeling. The calculation of secondary VDF follows the exact same strategy as the one for primaries: The VDF at a location of interest is assembled as a comprehensive scan in velocity space. Each individual velocity that is picked, determines a unique Keplerian trajectory along which the integration of secondary production terms is carried out. The secondary production calculation at an arbitrary point of the trajectory requires the knowledge of two collision partners, the helium ion and the neutral. The helium ion will become the secondary neutral after c.x., so it needs to be taken from a local plasma Maxwellian at exactly the velocity state that corresponds to what the neutral Kepler trajectory requires at that location. This gives an overall phase space density factor; often it is quite small because it represents a very improbable ion from the tail of the Maxwellian distribution, and overall strong secondary fluxes are only obtained when trajectory velocities coincide with the peak of local plasma Maxwelians. For simplicity, the width of the local He$^+$ Maxwellian (thermal velocity) is derived here from the local plasma temperature. As has been emphasized by, e.g., Zank et al. (1996, 2013), heliosphere plasmas are heated by charge exchange, yet the equilibration time scales are too long to allow an actual equilibration in the heliosphere, including in the outer heliosheath (Zank et al. 2014). The majority of global heliosphere models which track protons in the heliosphere as a single MHD fluid component, summarizes the contributions of thermal protons and non-thermal (such as pickup) ions in the form of a single, effective plasma temperature. The cooler thermal plasma component dominates by number and hence should be used for calculating charge exchange; using the effective plasma temperature currently systematically overestimates the width of the local He$^+$ Maxwellian. This issue will be addressed in future work.

For the other collision partner, i.e. the neutral atom, the neutral distribution function needs to be integrated in the form of a Boltzmann-style production integral, where the integrand depends on the relative neutral-ion velocity during the integration, as well as the cross section which itself depends on that relative velocity (e.g., Müller et al. 2000). Together with the standard loss calculation, the integration of the production terms yields the secondary phase space density at this investigated VDF velocity, at the point of interest under investigation. Scanning through all possible VDF velocities in this manner finally results in a complete secondary neutral VDF (example in section 3).

For the primary VDF calculations it was advantageous to determine first the locations of the peaks (both direct and indirect) in phase space density (PSD), and then obtain the VDFs in the velocity-vicinity of these peaks (Müller 2012; Müller & Cohen 2012). For the secondary VDF, this is not possible as it represents a distributed source rather than a “point” source at infinity. For this reason, the entire possible velocity space should in principle be scanned. In practice, one can however identify some promising velocity regions and hence restrict the velocity scanning.

The main production site for secondaries is the outer heliosheath. There is no production of secondaries upwind of the bow shock, and negligible production inside the heliopause. This
results in secondary VDFs whose maxima are quite close to the primary direct and indirect VDFs. Furthermore, there is a sharp cutoff toward lower velocities: For a given point of interest, there is a minimum velocity below which the total energy becomes negative, corresponding to closed, bound trajectories as opposed to the open ones that reach infinity and have non-zero kinetic energy even at infinity. Closed trajectories (Kepler ellipses) can still have aphelia that are distant enough to be in the outer heliosheath and beyond and therefore have secondary production along parts of their trajectory. When the aphelia are interior to the heliopause, then there are practically no secondaries produced along the entire orbit, leading to a precipitous drop in phase space density (PSD) for these velocities. This criterion forms a sphere in velocity space around the origin; the spherical volume within has practically zero secondaries, and there is no need to scan this velocity volume (which of course also lacks primaries). For this reason, the scan strategy for the secondary VDF is carried out in spherical polar coordinates in velocity, with the inner radius (minimum velocity) as outlined. Far away from direct and indirect primary peaks, the secondary VDF also drops to very low levels, hence the scanning strategy stops at an outer radius (maximum velocity). For more comprehensive studies, VDF scanning should be carried further to velocities that correspond to solar wind velocities, to identify side peaks in the neutral secondary VDF generated by double charge exchange of solar wind alpha particles (second c.x. reaction listed in section 2.1).

3. Results and Discussion

As a sample of the viability and the success of the method outlined above, Figure 1 contains results representing the secondary neutral helium VDF at a location of interest (0,1) that is 1 AU from the Sun. The location is perpendicular to the ISM flow. While the actual VDF is an object in three-dimensional velocity space, Figure 1 presents a 2D slice through it, at a central slice plane that contains the peaks of the VDF.

The figure shows the concept of the VDF not having been calculated inside of a minimum velocity (here, about 40 km/s); this entire region represents closed ellipses that do not reach outside of the heliopause and therefore do not contain any secondary production terms. As can be seen from the phase space densities both in color and as contour lines, the transition to this regime is quite steep, which is an indication that the aphelion distance is a steep function of velocity magnitude here.

In the velocity region indicated by the inner and outer circular bounds (a thick velocity shell in 3D), the black contour lines identify the primary direct VDF, peaking at (-45, -20) velocity which is the ISM velocity vector (-26.3, 0) transported into the solar gravity well to the point (0, 1), and the primary indirect VDF peaking at (20, 45) which corresponds to particles that have run from the ISM through perihelion and were on their way out when they intersected with the location (0, 1). Losses for the indirect peak are stronger because of the trip around the Sun, resulting in depletion so that the normalized phase space density $f = 0.1$ contour is already missing (the respective outermost contours correspond to $f = 10^{-4}$; all these numbers are normalized so that the PSD in the pristine LISM is 1).

The color scheme represents the secondary neutral He phase space density with the same normalization as the primary one, i.e. directly comparable to the primaries. The color map spans 5 orders of magnitude, and starts where the primary contours end. The secondary PSDs are quite low, yet they organize themselves in the vicinity of the direct and indirect primary peaks. Because of the general nature of secondaries being slower, it makes sense that the secondary peaks occur at lower velocities, (-34, -25) for the direct secondary peak and (29, 32) for the indirect secondary peak. The appearance also confirms that secondaries are more deflected when compared to primaries. The actual peak value for the direct secondary peak is $f_2 = 2.8 \times 10^{-5}$ (for the indirect, $f_2 = 3.4 \times 10^{-6}$). These numbers, which are normalized to the neutral helium PSD in the LISM, are quite low; a recent IBEX analysis determined secondary flux levels to be
Figure 1. Example calculation of primary (black contours, $f$) and secondary (color contours, $f_2$) particle distributions at the point (0,1) sidewind, for one particular global heliospheric model. The values are normalized to the primary LISM value. While the secondary neutrals are at lower densities, their addition to the overall VDF still yields a shift in bulk velocity and temperature. The inner cutoff radius expresses a speed for which trajectories no longer connect with the outer heliosheath.

5.7% of the interstellar primary value (Kubiak et al. 2016). The discrepancy between the ab-initio model of secondaries presented here and the IBEX observations deserves future attention, including the exploration of the parameters of Table 1 and of the other assumptions made for this initial version of the calculations.

A modeled trajectory in the actual code that represents the secondary direct peak particles of Figure 1, enters the global background simulation domain at location (1000 AU, -28 AU) with a positive $v_y$ component, traverses the outer heliosheath on a trajectory close to the symmetry axis and essentially parallel to the shocked plasma, runs through the point of interest (0, 1), experiences a perihelion at $r = 0.66$ AU, and exits the simulation domain on the outgoing hyperbola leg at location (780 AU, -620 AU).

Around the direct peak, the primary and secondary levels become comparable, at least away from the primary peak, which supports the statement that secondaries have the potential to disguise as tails of the primaries and hence throw off the analysis of the primaries when
secondaries are neglected. The addition of the secondary component to the primary VDF can shift and broaden the overall VDF. These parameter changes will depend on the location of interest.

Once the combined He velocity distribution is known at the location of the spacecraft, a simulated He flux map, comprised of both primaries and secondaries, can be computed for comparison with the observations. This simulated flux map must take into account the energy efficiency and detector geometry function for the spacecraft detector involved. It will be the comparison of synthesized with measured fluxes from Ulysses and IBEX that will allow a determination of the plasma characteristics of the outer heliosheath through model parameter variations and identifying the best match between model and experiment.

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