Modeling heavy ions and atoms throughout the heliosphere

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Abstract. Most investigations addressing the global structure of the heliosphere, including explicitly the interaction between the solar wind and the partially ionized local interstellar medium (LISM), have focused on hydrogen since it is the most abundant particle species. We use kinetic models that include heavy elements such as He, C, N, O, and others, to study the heliospheric distribution of neutrals and the singly charged ions of these species, besides H. Our model describes the evolution of interstellar heavy neutral atom distributions throughout the heliosphere, and we include the interaction of heavy particles with neutral hydrogen and protons through charge exchange (i.e., the creation of pickup ions), while the heavy particles are subject to photoionization and gravity. We use improved, recently published charge exchange cross-sections as well as recently identified LISM boundary conditions. A realistic description of the basic heavy element distribution and filtration at heliospheric boundaries will provide an important theoretical basis for interpreting observations of pickup ions made by Ulysses and ACE.

INTRODUCTION

The interaction of the ionized solar wind with the partially ionized local interstellar medium (LISM) defines the heliosphere with its characteristic boundaries, the termination shock and the heliopause. The dominant particle species are neutral hydrogen (H) and its atomic constituents, protons and electrons. Consequently, numerical models to study the global heliosphere focus on the self-consistent modeling of the interaction of solar wind hydrogen plasma with the LISM hydrogen wind which consists of both neutral H and hydrogen plasma. The consideration of neutral H in the heliosphere is an important ingredient of heliospheric physics since the coupling of neutral H to the plasma via charge exchange affects the plasma distribution profoundly, which in turn feeds back to the neutral H distribution.

The solar wind and the LISM contain elements heavier than hydrogen as well. The direct solar wind includes heavy ions in various high charge states. In addition, there are sources for neutral heavy atoms in the inner heliosphere, such as the “inner source” (likely released from dust) and planetary atmospheres. However, the LISM provides a much higher density of neutral atoms. These interstellar atoms can penetrate through the heliospheric boundaries into the inner heliosphere, where they, together with the corresponding pickup ions, serve as messengers from the LISM which is currently out of reach for in-situ measurements.

In order to gain an understanding of the LISM through the measurement of neutral heavy atoms and their singly charged heavy ions, it is necessary to know what changes the interstellar neutral atom population undergoes on its path through the heliosphere. The dominant interactions are the charge exchange of a neutral atom with the plasma proton background, \( A + p \rightarrow A^+ + H \), creating a singly charged heavy pickup ion, and the reverse process, \( A^+ + H \rightarrow A + p \) which creates a neutral heavy atom. These two processes let the hydrogen background influence the heavy interstellar elements in the heliosphere. In addition, heavy atoms will experience photoionization close to the Sun, as well as gravity.

MODEL

In this study, we first model a complete hydrogen heliosphere, with an assumed steady solar wind with density \( n_p = 5 \text{cm}^{-3} \), velocity \( v = 400 \text{km s}^{-1} \), and temperature \( T = 10^5 \text{K} \) at 1 AU. The interstellar hydrogen velocity is set to \( v = 26 \text{km s}^{-1} \). The density and temperature are less well known, and we use two sets of values, namely, a low-density, high-ionization fraction background model 1 with \( n_H = 0.14 \), \( n_p = 0.1 \text{cm}^{-3} \) and \( T = 8000 \text{K} \), and the alternative background model 2 with \( n_H = 0.216 \), \( n_p = 0.047 \text{cm}^{-3} \) and \( T = 7000 \text{K} \). The hydrogen distributions are modeled with a multifluid code [1], and representative plots for plasma temperature and neutral H number density are given in Figures 1 and 2. Both cases have a pronounced hydrogen wall between heliopause and bow shock, with neutral densities reaching peaks of 2.3 times above their respective interstellar neutral
differences. While the locations of termination shock and heliopause shift in response to the different interstellar ionization fraction, the filtration ratios at the termination shock (the amount of neutral H reaching the TS, compared to the interstellar density of neutral H) are similar (0.40 and 0.46, respectively). In absolute terms, of course, there is much more neutral H present in the background model 2 throughout the heliosphere, and correspondingly more pickup protons are produced.

With the hydrogen as a background, we model the flow of interstellar neutral heavy atoms and singly charged heavy ions into and around the heliosphere. We use a kinetic direct Boltzmann solver (modified from [2, 3, 4]) that tracks the two species through trajectories of macroparticles while exchanging charge with the hydrogen background, and while being affected by photoionization and gravity.

The focus of this study are the elements N and O, as well as the noble gases He, Ne, and Ar. Pickup processes with these elements in the heliosphere are relevant for processes leading to anomalous cosmic rays. All these elements are present in the ISM both in neutral and ionized form. We additionally study carbon which is almost completely ionized in the LISM. For the quantitative boundary values, we use the number densities given in Table 1. They are derived from model 17 of Slavin & Frisch [5] who model the nearby ISM taking into account measured column densities along different sightlines and models for the radiation environment of the Local Interstellar Cloud. As can be seen from Table 1, among the six elements mentioned here only Ne and Ar have a significant density of charge state larger than 1.

The Slavin & Frisch [5] calculations leading to model 17 also give an estimate for the interstellar H densities, which we did not use here for our background model. Their neutral hydrogen value is similar to background 2, and the proton density is similar to the one of background 1. Therefore, while the LISM hydrogen boundary values assumed in the present study are not self-consistent with the rest of the elemental densities, the two H background models used here straddle the Slavin & Frisch H values.

### RESULTS

Figures 3–5 show typical heavy atom (left) and ion (right) distributions resulting from the two-dimensional kinetic models. Direct interstellar ions are excluded from entering the heliosphere. The interior heliosphere is left with a very low density of ions created from neutrals via charge exchange (pickup ions). The heliopause, created by hydrogen, bounds this depleted cavity. The stagnating flow of H plasma upwind of the heliopause translates into a deceleration and density enhancement of the heavy ions as well [6].

The charge exchange cross section of (He, H) and (O, H) are very different, both in the way they depend on the particle energy, and in magnitude, with the helium exchange cross section lower than that of oxygen. This fact finds its most prominent expression in the appearance of a neutral oxygen wall [7] upwind of the heliopause (Figure 4), whereas neutral helium traverses the heliospheric boundaries practically unimpeded, with only a focusing downwind of the Sun due to gravity that is not balanced.
FIGURE 3. Neutral and singly ionized oxygen (model against H background 1), shown through neutral density (left) and ion density (right, in cm$^{-3}$).

FIGURE 4. Same as Fig. 3, for hydrogen background 2.

FIGURE 5. Neutral and singly ionized helium (model against H background 2), shown through neutral density (left) and ion density (right, in cm$^{-3}$).

TABLE 2. Model results for H backgrounds 1 and 2.

<table>
<thead>
<tr>
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<th>filtration upwind TS</th>
<th>filtration downwind TS</th>
<th>amplification in wall</th>
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<td>1</td>
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by radiation pressure (Figure 5). A similar focusing occurs also for oxygen. The oxygen wall feeds back to the oxygen plasma so that the ion enhancement upwind of the heliopause is even more pronounced than for helium.

When comparing the oxygen 2D density maps for two distinct H background models in Figures 3 and 4, the size differences are obvious and relate to the H background (Figures 1 and 2). In addition, because of the larger H densities in background model 2, the corresponding neutral oxygen wall has a larger maximal value. Figure 6 shows the number density profiles along the LISM flow symmetry axis (with Sun at 0) for all 6 modeled element species using H background 2. The bold lines represent the neutral number density, while the thin dashed lines are pickup and interstellar heavy ion densities. The locations of termination shock TS, heliopause HP, and bow shock BS of the heliosphere are marked in the oxygen panel. While on the order of $10^7$ particles in the simulations produce reasonable statistics in most parts of the profiles, the scarcity of pickup ions results in substantial statistical noise for their part in the ion density curves.\footnote{The simulations with H background 1 have been done with fewer particles, resulting in a higher level of graininess in Figure 3.}

As is evident from Figure 6, only oxygen, and to a lesser extent nitrogen due to its charge exchange cross section dependence on energy similar to that of oxygen, has a wall-like neutral density enhancement upwind of the heliopause. The neutral helium density is basically constant on the chosen scales. Ne, Ar, as well as C do not show an enhancement in the form of a wall, but exhibit depletion close to the Sun on the upwind side, and refilling of the ionization cavity due to focusing on the downwind side. For the singly ionized heavy interstellar particles, there is a density enhancement upwind of the heliopause, as already discussed above.

Table 2 summarizes some results obtained from the two sets of heavy elements models. The filtration ratios for the upwind termination shock location are important for all calculations of pickup ion densities in the inner
The heliosphere, and as input for ACR acceleration processes at the TS. The filtration ratios for the downwind TS are given as an illustration of the depletion of neutral atoms while they traverse the region of the supersonic solar wind. Lastly, the amplification in the wall is an expression of the peak density of neutral heavy atoms just upstream of the heliopause.

The results given in Table 2 support the discussions above. He, C, and N do not experience appreciable filtration, and Ne and Ar only a modest amount. The models predict even a small enhancement for neutral oxygen. However, this result might not hold up when additional ionization processes, such as electron impact ionization, are considered in future models. The downwind TS values are about the same across the elements, with the exception of He which owes its better survival to the lower photoionization rate assumed here. The neutral atom walls upwind of the heliopause behave as discussed above, with the exception of a slight, unexpected overdensity of helium for background model 1.

Table 2 also allows for an estimate of how sensitive such heavy element calculations are to the assumed hydrogen background. Comparing adjacent columns of Table 2 to each other, there is an overall agreement, indicating somewhat low sensitivity to the H background. As expected due to their larger charge exchange cross sections, nitrogen, and even more so oxygen, do react to changes in the H background, with upwind filtration and amplification values varying here by \( \sim 10\% \). In general, the filtration ratio seems to depend on the H background on that level, with the notable exception of helium.

In summary, the results emphasize the importance of the charge exchange cross sections to the filtration and distribution of interstellar neutral heavy atoms in the heliosphere. Elements weakly coupled to H experience only modest losses when traversing the heliosphere, and filtration is not sensitive to the details of the H background. Elements coupled more strongly to H, such as O and N, are sensitive to the background H distribution, and react more strongly in the form of neutral walls and changed filtration ratios.

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