The Evolution of the Large-scale ISM: Bubbles, Superbubbles and Non-Equilibrium Ionization

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Abstract. The ISM, powered by SNe, is turbulent and permeated by a magnetic field (with a mean and a turbulent component). It constitutes a frothy medium that is mostly out of equilibrium and is ram pressure dominated on most of the temperature ranges, except for $T < 200$ K and $T > 10^6$ K, where magnetic and thermal pressures dominate, respectively. Such lack of equilibrium is also imposed by the feedback of the radiative processes into the ISM flow. Many models of the ISM or isolated phenomena, such as bubbles, superbubbles, clouds evolution, etc., take for granted that the flow is in the so-called collisional ionization equilibrium (CIE). However, recombination time scales of most of the ions below $10^6$ K are longer than the cooling time scale. This implies that the recombination lags behind and the plasma is overionized while it cools. As a consequence cooling deviates from CIE. This has severe implications on the evolution of the ISM flow and its ionization structure. Here, besides reviewing several models of the ISM, including bubbles and superbubbles, the validity of the CIE approximation is discussed, and a presentation of recent developments in modeling the ISM by taking into account the time-dependent ionization structure of the flow in a full-blown numerical 3D high resolution simulation is presented.

1. Introduction

In the last decade due to the substantial increase of computing power, sophisticated models of the interstellar medium (ISM), including the disk-halo interaction, bubble and superbubble evolution, molecular clouds evolution and fragmentation, formation of shock compressed layers, etc., in a turbulent supernova-driven medium, have been developed. In general these models included cooling and heating, which determine the physical state of the gas. Interstellar cooling can be the result of line and continuum plasma emission processes, as well as of adiabatic expansion of over-pressured gas. The importance of the former depends on the amount of atoms and ions present in the flow, whereas the latter is related to thermodynamical processes. For optically thin interstellar plasmas, frequently the assumption of collisional ionization equilibrium (CIE) is used, according to which the collisional excitation of the gas is followed by photon emission, with the number of ionizations being equal to the number of (dielectronic or radiative) recombinations. However, CIE violates detailed balancing, since collisional excitation involves three particles, an atom or ion, an electron to collide with, and a second electron which is ejected, whereas in radiative recombination, the third particle...
is a photon, leaving the system. Thus, strictly speaking, CIE can never be maintained in an evolving plasma, although it might be a fair approximation, especially in hot (T > 10^6 K) environments. For lower temperatures recombinations are not synchronized with the cooling and therefore, deviations from CIE inevitably occur (see e.g., Kafatos [1973], Shapiro, & Moore [1976], Schmutzler & Tscharnuter [1993]).

The CIE assumption in all ranges of temperatures, or at least in part of it, in the models discussed below implies the use of a specific cooling function, for given abundances, in the computational domain and at each time step. Obviously, the history of the ionization structure, which depends on the thermodynamic path of the plasma, will be lost, in contrast to a full non-equilibrium ionization (NEI) structure giving rise to a time-dependent cooling function, which is quite different than that obtained under CIE conditions.

The structure of this paper is the following: In Section 2 a review on ISM modelling including superbubbles and disk-halo interaction, is presented. Sections 3 and 4 deal with the collisional ionization conditions adopted in the models, and compare CIE with NEI results, respectively. As cooling is a process that depends on the history of the plasma, we discuss in Section 5 the cooling functions and emission spectra of gas in the latest simulations of the ISM. The paper is closed with a final remarks and conclusions section.

2. From the 3-Phase Model to Present day ISM and Superbubbles Models

Theoretical studies during the last three decades have culminated in the supernova regulated Interstellar medium models of Cox & Smith (1974) and in the widely accepted “standard-model” (McKee & Ostriker 1977), in which the gas is distributed into three phases in global pressure equilibrium, a cold and warm neutral phase (CNM and WNM, respectively), a warm ionized (WIM) and a hot intercloud (HIM) medium. There is global mass balance by evaporation, ionization and condensation, and energy balance between supernova (SN) energy injection and radiative cooling. Most of the Galactic volume (up to 70-80%) is filled with the hot (> 10^5 K) low-density (~ 10^{-3} cm^{-3}) ionized gas, interspersed by cold neutral and relatively dense clouds. Observationally it was difficult to determine reliable volume filling factors of the hot phase in our Galaxy due to the observational vantage point. However, it became evident that the small surface coverage of H_i holes in external galaxies (e.g., Brinks & Bajaja [1986]) argues for a much lower volume filling factor of the hot phase there.

Furthermore, Population I stars typically born in OB associations (see, e.g., McCray & Snow [1979], McCray & Kafatos [1987]). Since more massive stars evolve more rapidly than low mass stars, the associations still exist when the first SNe occur. Hence, SNe are not randomly distributed over the entire galaxy. As a result of their motions, up to 40% of the stars explode in the field (see review by Ferrière [2001]). Therefore, the amount of hot gas will mostly be concentrated in isolated pools (forming superbubbles), which may burst through the thick disk (composed of H_i (Lockman [1984]) and H_ii (Reynolds [1985] layers) into the halo like chimney funnels (Norman & Ikeuchi [1989]). The superbubble evolution in a static density stratified environment was modelled hydrodynamically in two dimensions by, e.g., Tomisaka & Ikeuchi [1986], Mac Low et al. [1989], and Tenorio-Tagle et al. [1990]. Tomisaka [1998] and Stil et al. [2009] developed three-dimensional simulations of a superbubble evolving in a static magnetized
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medium having a stratified structure along the direction perpendicular to the Galactic midplane.

With the presence of such an extended thick disk, arguments were put forward that the break-out of bubbles and superbubbles could be inhibited (unless they occurred at a significant height above the disk) and only the most energetic superbubbles (SBs) would achieve blow-out of the disk (see [Koo & McKee 1992]). Things might even become worse as superbubble (SB) break-out may be inhibited by a large-scale disk parallel magnetic field (e.g. Mineshige et al. 1993; Tomisaka 1998). On the other hand, it seems paradoxical that terrestrial plasmas are so hard to confine, whereas ISM plasmas should be magnetically tied down to the disk. In fact in both cases small and large scale instabilities destroy the highly symmetric configuration, like e.g. the Parker (1966) instability in the astrophysical context. Observationally, owing to the high sensitivity and large throughput of the ROSAT XRT (Trümper 1983) and its PSPC instrument, a number of normal spiral galaxies with soft X-ray halos were detected, e.g. NGC 891 (Bregman & Pildis 1994) and NGC 4631 (see Vogler & Pietsch 1996). In some cases, even local correlations between Hα, radio continuum and soft X-rays were found (Dettmar 1992), arguing for local outflows as it had been suggested in the Galactic fountain (Bregman 1980; Kahn 1981), chimney (Norman & Ikeuchi 1989) and the Galactic wind model (Breitschwerdt et al. 1991; Breitschwerdt & Schmutzler 1994).

These models capture some of the structure but not all of the essential physics. Taking into account that the ISM is a turbulent and compressible system (von Weizsäcker 1951), in which cooling and heating determine the physical state of the gas, more complex and sophisticated galactic disk (two-dimensional: Chiang & Prendergast 1985; Chiang & Bregman 1988; Rosen et al. 1993; and disk-halo interaction two- (Rosen & Bregman 1995) and three-dimensional (Korpi et al. 1999a; Avillez 2000; Avillez & Breitschwerdt 2004; 2005; Joung & Mac Low 2006; Melioli et al. 2009) models were developed. In turn, some of these models have been used to follow the evolution of superbubbles within a realistic supernova-driven turbulent magnetized medium (in contrast to previous simulations that used a static medium) by Korpi et al. (1999b) and Avillez & Breitschwerdt (2005) (a field composed of a random and mean components with a total strength of 4.5 µG was used) finding that blow-out is much more likely than previously thought, mainly because bubbles evolve in an inhomogeneous background medium. However, Korpi et al.’s simulations are limited by the usage of a small grid extending only up to 1 kpc in the direction perpendicular to the disk in both sides of the midplane. Hence, the disk-halo-disk cycle could not be established nor followed.

The simulations of Melioli et al. (2009) calculate the time evolution of Hα, Hν, Cii–Civ, and Oi–Oiii ions at T ≤ 10⁶ K and determine their contributions to the cooling function. For T > 10⁶ K they use a CIE cooling curve. Such setup has severe implications in the history and cooling of the plasma as will be discussed below.

The evolution of superbubbles can be much improved by, instead of injecting energy in a continuous way into a single point, identifying the missing stars in an association and follow in space and time all the stars during their main sequence life time until they explode. This methodology has been used in the disk-halo simulations, including those related to the evolution of the Local and Loop I superbubbles in a turbulent medium (Breitschwerdt & Avillez 2006; Avillez & Breitschwerdt 2009). In this way one can perform a detailed simulation of the properties of the bubbles and their spectroscopic observables, allowing a direct comparison with observations. These simulations
have been successful in reproducing not only the spatial structure of the bubbles, but also the observed column densities of Li-like ions C\textsc{iv}, N\textsc{v} and O\textsc{vi} and their ratios.

3. Plasma Emission Modelling

A further improvement in modelling the ISM comprises the full-blown non-equilibrium ionization structure (resulting from the ten most abundant elements), where the ionization, thermal and dynamical history of the plasma are fully nonlinearly coupled and tracked simultaneously both in space and time at high resolution. In order to achieve this, we developed a plasma emission code (hereafter EPEC - Eborae Plasma Emission Code) which can be coupled to any MHD software through the proper interfacing calls. EPEC is written in Fortran 2003 in an object-oriented way making large use of procedure pointers. It is prepared to run both on multi-core CPUs (using OpenMP) as well as on NVIDIA GPUs (graphics cards processor units) by means of CUDA Fortran.

3.1. Abundances

EPEC includes the ten most abundant elements in nature (H, He, C, N, O, Ne, Mg, Si, S and Fe) and the default solar abundances are those recommended by Asplund et al. (2009, AGSS2009): \( \log A(X/H)_{\odot} = -1.07 \) (He), -3.57 (C), -4.17 (N), -3.31 (O), -4.07 (Ne), -4.40 (Mg), -4.49 (Si), -4.88 (S), and -4.50 (Fe). Other abundances (for comparison studies with previously published results) are also available, e.g., Allen (1973), Anders & Grevesse (1989, AG1989) and Grevesse et al. (2007, GAS2007). The latter are used by Gnat & Sternberg (2007), but with the Ne overabundance (\( \log A(Ne/H)_{\odot} = -3.71 \)) of Drake & Testa (2005). GAS2007 and AGSS2009 propose C, N, O and Ne abundances smaller than those recommended by AG1989, but AGSS2009 increases slightly those values from GAS2007. This variation in the abundances results from the improvement on three-dimensional hydrodynamical solar model atmospheres, that include a relaxation assumption on the local thermodynamic equilibrium and improvements in the atomic and molecular data (see discussion in, e.g., AGSS2009).

3.2. Atomic and Cooling Processes

The adopted physical processes in this work are the electron impact ionization, excitation-autoionization, radiative and dielectronic recombination, charge-exchange recombination and ionization reactions, continuum and line emissions. Electron impact ionization rates fits are taken from Mattioli et al. (2007, MAT2007) for all H, He, C, N, O, Ne ions, Mg-I-Mgiii, Si-i-Sivii, Si-Sv, and Fe-I-Fexi; The experimental data of Fogle et al. (2008) is used to fit the rates for Cii, Niv, and Ov. Data for the remaining ions is taken from Mazzotta et al. (1998, MAZ1998). Excitation-autoionization rates are taken from MAT2007 for C\textsc{iv}, N\textsc{v}, O\textsc{vi}, Ne\textsc{vii}, Si\textsc{iii}-Si\textsc{iv}, S\textsc{ii} and Fexi. For the remaining ions where EA is important we follow Arnaud & Rothenflug (1985, AR85).

Radiative recombination rates are fitted following Verner & Ferland (1996) and Gu (2003), for low charge ions. The fits parameters for bare through Na-like ions are taken from Badnell (2006) and for other ions we follow Dere et al. (2009). Dielectronic recombination rates fits coefficients for H-like through Mg-like ions are taken from Badnell (2006), Zatsarinny et al. (2003, 2004, 2006 and references therein), Colgan et al. (2003, 2004), Altun et al. (2004, 2006, 2007), Mitnik & Badnell (2004) and Bautista & Badnell (2007) with updates for Svi (Orban et al. 2009), Nevi (Orban et al. 2008),
Fevn-Fex (Schmidt et al. 2008), Fex-Fexi (Lestinsky et al. 2009), Fexyv (Schmidt et al. 2006), Fexv (Lukic et al. 2005), Fexxi (Savin et al. 2006). For the remaining ions MAZ1998 data is used.

Charge-exchange recombination (CER) with H\textit{i} rates for H\textit{e}n-H\textit{e}ii, N\textit{u}-N\textit{v}, O\textit{m}, O\textit{v}, Ne\textit{u}-N\textit{v}, Mg\textit{m}-Mg\textit{v}, Si\textit{v}-Si\textit{v}, and Fe\textit{n}-Fe\textit{xv} are taken from Kingdon & Ferland (1996), Cu-Cm (Suno & Kat0 2006), O\textit{v} (Wang et al. 2003), Si\textit{ii} (Clarke et al. 1998), and Si\textit{v} (Bruhns et al. 2008). Fits to the rates of CER with H\textit{e} for N\textit{u}-N\textit{v}, O\textit{m}, O\textit{v}, Ne\textit{u}-N\textit{v}, Cm-Cm, Mg\textit{m}-Mg\textit{v}, Si\textit{v}-Si\textit{v}, Si\textit{v} and Fe\textit{n}-Fe\textit{xv} are taken from Astrophysics Charge-Transfer Database (Wang et al. 2002a, and references therein). O\textit{v} (Zhao et al. 2005), O\textit{v} (Wu et al. 2009), Ne\textit{m} (Zhao et al. 2006), Si\textit{ii} (Zhao et al. 2005), Si\textit{v} (Wang et al. 2002b), and Fe\textit{n}-Fe\textit{xv} (Cadez et al. 2003). Charge-exchange ionization (CEI) with H\textit{i} rates for Mg\textit{m}, Si\textit{v}-Si\textit{v} are taken from AR1985, C\textit{i}, N\textit{i}, Mg\textit{i}, Si and Fe\textit{n}-Fe\textit{i} are taken from Kingdon & Ferland (1996) and O\textit{v} from Spiro et al. (2003). CEI with H\textit{e}n comprised data for O\textit{v} (Zhao et al. 2004) and Si\textit{v} (Wang et al. 2002b), C\textit{i}, N\textit{i}, Si\textit{v} and Si\textit{v}-Si\textit{v} (AR1985).

Cooling rates include free-free emission with the averaged Gaunt factor by Karzas & Latter (1961), radiative and dielectronic recombination (Cox & Tucker 1969), line emission in the range 1 Å -610 \( \mu \) (Penston 1970; Jura & Dalgarno 1972; Dalgarno, & McCray 1972; Kato 1976; Stern et al. 1978; Gaetz & Salpeter 1983; Mewe et al. 1985), and two-photon emission. Spectra calculations include line and continuum emissions. The latter comprises free-free, free-bound to the ground and excited states, and two-photon, using 1s-2s transitions in H and He-like ions (Tucker & Gould 1966; Gronenschild & Mewe 1978; Mewe et al. 1986).

3.3. Equations

The time evolution of the ions fractions, where ionization and recombinations of ions of nuclear charge \( Z \) occur between neighbouring ionization stages \( z - 1 \), \( z \) and \( z + 1 \), is given by

\[
\frac{dn_{Z^z}}{dt} = I_{Z^z-1} n_{Z^z-1} n_e - (I_{Z^z} + R_{Z^z}) n_{Z^z} n_e + R_{Z^z+1} n_{Z^z+1} n_e,
\]

where \( R_{Z^z} \) and \( I_{Z^z} \) are the rates of recombination and ionization from state \( (Z, z - 1) \) and \( (Z, z + 1) \), respectively; \( n_{Z^z} \) and \( n_e \) are the ion density of element \( Z \) with effective charge \( z \) and electron density, respectively. This constitutes a tridiagonal matrix if the charge exchange reactions are not included. However, if charge exchange reactions are included (as done in the present paper) new off-diagonals terms are introduced, becoming

\[
R_{Z^z} = \alpha_{Z^z}^r + \alpha_{Z^z}^d + \frac{1}{n_e} \sum \alpha_{Z^z}^{ef} \tilde{n}_{Z^z},
\]

where the uppers indices stand for radiative, dielectronic and charge exchange processes, respectively, and

\[
I_{Z^z} = C_{Z^z}^{ei} + C_{Z^z}^{ea} + \frac{1}{n_e} \sum C_{Z^z}^{ef} \tilde{n}_{Z^z},
\]

with \( eii \) and \( ea \) standing for electron impact and excitation-autoionization processes, respectively, and \( \tilde{n}_{Z^z} \) is the particle density of other ions involved in the charge exchange.
reactions. In the EPEC version referred to here, we do neither consider photoionization nor ionization due to suprathermal electrons (see, e.g., Schmutzler & Tscharnuter 1993) - this is the subject of a forthcoming paper. For the 10 elements considered in the EPEC, the number of ordinary differential equations including the neutrals amounts to 112. Conservation of species (atoms and ions) implies that

\[ n_{Z} = \sum_{z=0}^{Z} n_{Z,z}. \]  

(4)

In addition the system of equations must account for the mass

\[ n_{\text{tot}} = \sum_{Z} n_{Z} + n_{e} \]  

(5)

and charge conservations

\[ n_{e} = \sum_{Z} \sum_{z=1}^{Z} n_{Z,z} z. \]  

(6)

The system of equations is closed by the energy balance equation

\[ \frac{dU}{dt} - \frac{P}{n} \frac{dn}{dt} = -n_{e} n_{H} \Lambda \]  

(7)

where \( \Lambda \) is the cooling function, i.e., it represents the radiative losses per unit emission measure resulting from bremsstrahlung, radiative and dielectronic recombination, collisional ionization, line emission due to excitation, two-photon emission, and charge-exchange reactions. In these equations \( n_{H} \) is the hydrogen density and \( U \) is the internal energy density of the system. The internal energy comprises the contributions from thermal motions of the particles, represented by \( U_{\text{th}} \), and the potential energy associated with the ionization stages, that is the energy stored in or delivered from the high ionization stages of chemical elements (Schmutzler & Tscharnuter 1993). Hence, the internal energy density is given by

\[ U = U_{\text{th}} + \sum_{Z} \sum_{z=1}^{Z} \left( n_{Z,z} \sum_{z'=0}^{z-1} I_{Z,z'} \right), \]  

(8)

where \( I_{Z,z'} \) is the ionization potential of an ion with nuclear charge \( Z \) and effective charge \( z' \). The thermal part of the internal energy is linked to the pressure of the system through the equation of state \( P = (\gamma - 1) U_{\text{th}} \).

As initial conditions for static plasma calculations we assume a fully ionized gas at \( 10^{9} \) K. As the temperature decreases, recombination and ionization rates are calculated, following the simultaneous implicit calculation of the ionization fractions (including neutrals) and charge equation – implying the inversion of a \( 113 \times 113 \) matrix. Next the radiative losses, emission spectra and internal energy are calculated.

4. Collisional ionization Equilibrium vs. Non-Equilibrium ionization

Figure [1] shows the normalized cooling function of a static plasma (that is, with no dynamics included) that cooled from \( 10^{9} \) to \( 10^{2} \) K under CIE and NEI (isochorically)
conditions calculated with EPEC and using AGSS2009 abundances. Variations by factors of 6 at $10^{1.2}$ K are observed between the two efficiencies with the CIE cooling dominating over the NEI case between $10^{3.6}$ K and $10^{6}$ K (bottom panel of Figure 1). These variations are a consequence of the cooling efficiency due to the different emission processes (bremsstrahlung, radiative and dielectronic recombination, collisional ionization, line excitation and two-photon emission) being larger under CIE than NEI conditions for all elements taken into account. Figure 2 compares the contributions of these processes to the cooling per element (e.g., C, Ne and Fe) under CIE (top row) and NEI (bottom row) conditions.

For $T < 10^{4.1}$ K the cooling efficiency at the same temperature under NEI (isochoric) conditions is larger than in the CIE case as a result of the delayed recombination of the plasma. As recombination lags behind, single and double ionized species exist at lower temperatures (right column in Figure 3), something that does not occur under CIE, because ionization and recombination is synchronized, and therefore neutrals form at temperatures near $10^4$ K (left column in Figure 3).

While in CIE the ionization fractions (left panel Figure 3) depend only on the temperature and are sharply peaked, in NEI these same fractions (right panel Figure 3) depend on the dynamical and thermal history of the plasma. The higher ionization stages recombine to lower ones and eventually (when $T \sim 10^{3.8}$ K) only the lowest stages are abundant. However, the qualitative behaviour of all ionic stages is not the same. The highest ionic stages decrease continuously, that is, they always recombine to the next lowest stages, while the lowest stages increase continuously, that is the next highest stage recombines to them; the intermediate stages have two peaks resulting from the recombination of the next highest stage, but dielectronic recombination

![Figure 1](image1.png)

**Figure 1.** Top panel: Normalized CIE (dashed line) and NEI (solid line) cooling functions as function of temperature and calculated with AGSS2009 solar abundances. Bottom panel: CIE and NEI cooling functions ratio.
rapidly depletes it, leading to the formation of the next lower ionization stage. When dielectronic recombination is no longer effective, recombination from the next highest stage increases the ion amount. As soon as the highest stage is depleted, the next stage recombines to the next lowest stage.

These differences between CIE and NEI become quite noticeable in the emission spectra of the plasma at different temperatures (Figure 4). The spectra include line emission (cyan lines) and continuum (free-free (dashed black line), free-bound (green line) and two-photon (red line) emissions). With the decrease in temperature from $10^6$ to $10^{4.2}$ the CIE and NEI spectra become quite different as result of the free-bound emission dominating the spectra up to 500 Å at low temperatures. At high temperatures, above $10^6$ K the differences between the ionization structure under CIE and NEI conditions are small, and therefore the spectra in these two cases are similar. They
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Figure 3. Temperature variation of the ionization structure of C (top) and Ne (bottom) under CIE (left column) and NEI (right column) conditions for a gas cooling from $10^9$ K.

differ appreciably when the recombination lags behind, typically around $10^5$ K, with the continuum at low wavelengths (i.e., $\lambda < 100\textup{	extup{Å}}$) becoming free-bound dominated. Note that in the CIE case there is very little ($\ll 10^{-30}$ erg cm$^{-3}$ s$^{-1}$ Å$^{-1}$) emission with increasing range of wavelengths and decrease in temperature, e.g., at $10^5$ K: $\lambda < 73\textup{Å}$, $10^4.6$ K: $\lambda < 179\textup{Å}$ and $10^4.2$ K: $\lambda < 435\textup{Å}$. Hence, no X-ray emission is expected in the latter two cases under CIE unlike in NEI, where due to delayed recombination, there is emission to be expected in these ranges of wavelengths and temperatures (right panel Figure 4).

5. Signature of the Initial Conditions in the Turbulent ISM - NEI Modelling

In a turbulent supernova-driven ISM the state of the plasma, and therefore its ionization structure, is determined by the heating and cooling as well as by the flow dynamics. Hence, it is expected that the ionization structure of the plasma varies from place to place leading to a multitude of cooling functions in the computational box.

We carried out three-dimensional hydrodynamical disk-halo interaction simulations (in a patch of the Galaxy located at the solar radius with an area of $1 \textup{ kpc}^2$ parallel to the Galactic midplane, and extending to $\pm 10 \textup{ kpc}$ perpendicular to it, similar to those described in Avillez & Breitschwerdt (2007) using a resolution of $0.5 \textup{ pc}$ (the highest so far used for large scale ISM evolution) corresponding to an effective grid with $2000^3$ cells per $\textup{ kpc}^3$ boxes) and including (i) local self-gravity, (ii) heat conduction and (iii) time-dependent evolution of the ionization structure (of H, He, C, N, O, Ne, Mg, Si, S, and Fe) at each cell of the grid using EPEC described above; (iv) the revised solar
abundances by Asplund et al. (2009) are used; (v) Periodic boundary conditions are used along the vertical faces, while outflow boundary conditions are set at the top and bottom of the grid.

The left panel of Figure 5 displays the density distribution in the Galactic midplane at evolution time 400 Myr, while the right panel shows the regions with temperatures between $10^{4.9}$ K and $10^{6.1}$ K. The displayed time is long enough for (i) the signature of the initial plasma conditions at $t = 0$ to be wiped out (it takes some 80 Myr for this to happen; Avillez & Breitschwerdt 2004), (ii) the disk-halo-disk circulation to be fully established, and (iii) the system to reach dynamical equilibrium in a statistical sense (Avillez 2000, Avillez & Breitschwerdt 2004). The figure shows in great detail the topology of the frothy and turbulent ISM permeated with hot gas and having low temperature filamentary structures.

Bubbles and superbubbles dominate the landscape, but the volume filling factor (that is, the fraction of disk volume) of the hot gas is merely $\approx 20\%$ for the Galactic supernova rate. Dark blue regions have temperatures $\geq 10^7$ K resulting from recent supernova activity, whereas darkest red regions are molecular clouds with an excess density of $> 1000$ cm$^{-3}$ and temperature $T < 100$ K. Cold gas (red regions) is formed as a result of shock compressed layers and cooling instabilities in the flow. The details of these simulations due to the high resolution allow us to identify turbulent motions and their effects at small scales. Superbubbles and bubbles have turbulent flows of material
as can be seen in the cavities, which are crossed by sheet like structures with variable geometries. These turbulent flows are responsible for the redistribution of energy inside and outside of the cavities.

Because the plasma keeps a record of its history, and therefore, of its initial condition (temperature, total pressure and density - including mass fluxes from neighbouring locations), the ionization structure of the plasma varies from place to place leading to a multitude of cooling functions for the same initial temperature as can be seen in the left panel of Figure 6 which displays the cooling paths for gas having an initial temperature of $10^6$ K and located at sites K through O, respectively (shown in the right panel of Figure 5). The cooling efficiency fails to match that calculated under NEI (isochoric) conditions (black dashed line) all the way down to $10^2$ K (left panel of Figure 6), because the latter has less "potential energy" stored in high ionization stages.

An important consequence of this variability seen in the ionization structure evolution and cooling paths is the occurrence of X-ray emission, through free-bound transitions, at low temperatures, becoming larger than the corresponding NEI emission in a static plasma. The NEI spectra were calculated for a gas cooling in a time-dependent fashion from $10^9$ K. The right panel of Figure 6 shows that the free-bound emission from the K through O sites (red, green, blue, brown and magenta lines in the left panel) dominates the NEI (solid black line) and CIE (dashed black line) static plasma emission with decreasing temperature. This is a clear indication that recombination from the continuum is not following the cooling of the gas.

Figure 5. Left panel: Non-equilibrium ionization density distribution in the Galactic midplane at evolution time 400 Myr. The color scale refers to the logarithm of the number density. Cold (high density) gas is represented by red while hot (low density) gas is shown in blue. Right panel: Midplane gas temperature between $10^{4.9}$ and $10^{6.1}$ K at 400 Myr of evolution. The labels refer to a selection of sites having temperatures of $10^5$ K (labels A through E), $10^{5.5}$ K (labels F through J) and $10^6$ K (labels K through O).
6. Discussion and Final Remarks

In this paper we emphasize the importance in ISM simulations to follow the ionization structure of a plasma in a time-dependent fashion, coupled self-consistently to the dynamics. In fact, the circulation of gas between the disk and halo is a dynamic process, which involves a time scale, that can be much shorter than any of the microphysical time scales due to ionization and recombination. The gas escaping into the halo has an initial temperature well in excess of $10^6$ K, where the assumption of collisional ionization equilibrium (CIE) is approximately valid. As the hot plasma expands away from the disk it will cool adiabatically thereby reducing its temperature and density. The recombination of highly ionized species lags behind and occurs mainly at considerable heights from the disk.

New state of the art simulations of the ISM, focusing on the detailed description of the plasma ionization structure in a supernova driven ISM show that: (i) in a dynamic ISM, the ionization structure and, therefore, the cooling function, varies with time and from place to place, depending on the initial conditions and its history (a result in accordance to previous discussions by Kafatos (1973), Shapiro, & Moore (1976) and Sutherland & Dopita (1993) regarding static plasmas, i.e., with no dynamics included), (ii) the cooling path can be quite different for gas even with the same initial temperature, but having different densities and pressures, (iii) this path may not follow the one predicted by the pure plasma emission calculations, that is, without the dynamics included, and (iv) as a consequence, X-ray emission occurs at temperatures $< 10^5$ K. This is a consequence of the important emission contribution of delayed recombi-

![Figure 6](image-url)

Figure 6. **Left panel:** Normalized cooling functions at sites K through O shown in the right panel of Figure 5 having an initial temperature of $10^6$ K. **Right panels:** Free-bound emission (color curves) from gas having an initial temperature of $10^6$ K, located at sites K-O and having the cooling curves displayed in the left panel. Solid and dashed black lines represent the emission expected from NEI and CIE static (i.e., no dynamics) plasma at the temperatures shown in each panel.
nation, arising from a severe mismatch of recombination and dynamical time scales of the plasma. Hence, as $T$ decreases, the emissivity becomes much larger, by more than an order of magnitude, than that predicted by CIE at the same temperature.

A fundamental consequence of the previous discussion, is that the cooling at any point in the ISM depends clearly on the history and dynamics of the plasma, that is, the ionization structure keeps a record of its initial conditions and the thermodynamic path it has taken. As the ionization structure varies from place to place there exists a multitude of different cooling functions in the ISM. Furthermore, with delayed recombination having an important role in the cooling of overionized gas, i.e. gas which once had a high temperature during its history, X-ray emission at low temperatures is expected. Consequently, the mismatch of observed plasmas, e.g. by DXS (Sanders et al. 2001), XQC (McCammon et al. 2002), EUVE (Jelinsky et al. 1995), with standard CIE emission models (even for multi-temperature fits) may eventually result from not correctly describing the NEI structure of the plasmas.

In addition, the amount of singly ionized ions which are important for molecular cloud chemistry, will also be affected by the timescales for recombination and cooling paths. This implies that a careful study of the ionization structure at higher temperatures is needed when one is dealing with molecular chemistry in the ISM.

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References
Allen, C. W. 1973, Astrophysical Quantities, 3rd ed., Athlone Press, London
Altun, Z., Yumak, A., Badnell, N. R., Colgan, J., & Pindzola, M. S. 2004, A&A, 420, 775
Altun, Z., Yumak, A., Badnell, N. R., Loch, S. D., & Pindzola, M. S. 2006, A&A, 447, 1165
Altun, Z., Yumak, A., Yavuz, I., et al. 2007, A&A, 474, 1051
Anders, E., & Grevesse, N. 1989, Geochim. Cosmochim. Acta, 53, 197
Arnaud, M., & Rothenflug. R. 1985, A&AS, 60, 425
Asplund, M., Grevesse, N., Sauval, A. J., & Scott, P. 2000, ARA&A, 47, 481
Avillez, M. A. 2000, MNRAS, 315, 479
Avillez, M. A., & Breitschwerdt, D. 2004, A&A, 425, 899
Avillez, M. A., & Breitschwerdt, D. 2005, A&A, 436, 585
Avillez, M. A., & Breitschwerdt, D. 2007, ApJ, 665, L35
Avillez, M. A., & Breitschwerdt, D. 2009, ApJ, 697, L158
Badnell, N. R. 2006, A&A, 447, 389
Bautista, M. A., & Badnell, N. R. 2007, A&A, 466, 755
Bregman, J. N. 1980, ApJ, 236, 577
Bregman, J. N., & Pildis, R. A. 1994, ApJ 420, 570
Breitschwerdt, D., McKenzie, J. F., & Völk, H. J. 1991, A&A 245, 79
Breitschwerdt, D., & Schmutzler, T. 1994, Nature 371, 774
Breitschwerdt, D., & Avillez, M. A. 2006, A&A 452, L1
Brinks, E., & Bajaja, E. 1986, A&A 169, 14
Bruhns, H., Kreckel, H., Savin, D. W., Seely, D. G., & Havener, C. C. 2008, Phys. Rev. A, 77, 64702
Čadež, I., Greenwood, J. B., Lozano, J., Mawhorter, R. J., Niimura, M., Smith, S. J., & Chutjian, A. 2003, J. Phys. B.: At. Mol. Opt. Phys., 36, 3303
Chiang, W.-H., & Prendergast, K. H. 1985, ApJ, 297, 507
Chiang, W.-H., & Bregman, J. N. 1988, ApJ, 328, 427
Clarke, N. J., Stancil, P. C., Zygelman, B., & Cooper, D. L. 1998, J. Phys. B.: At. Mol. Opt. Phys., 31, 533
Colgan, J., Pindzola, M. S., Whiteford, A. D., & Badnell, N. R. 2003, A&A, 412, 597
Colgan, J., Pindzola, M. S., & Badnell, N. R. 2004, A&A, 417, 1183
Cox, D. P., & Tucker, W. H. 1969, ApJ, 157, 1157
Cox, D. P., & Smith, B. W. 1974, ApJ, 189, L105.
Dalgarno, A., & McCray, R. A. 1972, ARA&A, 10, 375
Dere, K. P., Landi, E., Young, P. R., Del Zanna, G., Landini, M., & Mason, H. E. 2009, A&A, 498, 915
Dettmar, R.-J. 1992, Fund. of Cosm. Phys. 15, 143
Drake, J. J., & Testa, P. 2005, Nature, 436, 525
Ferrière, K. 2001, Rev. Mod. Phys., 73, 1031
Fogarty, M., Bahati, E. M., Bannister, M. E., et al. 2008, ApJS, 175, 543
Gaetz, T. J., & Salpeter, E. E. 1983, ApJ, 52, 155
Gnat, O., & Sternberg, A. 2007, ApJS, 168, 213
Gronenschild, E. H. B. M., & Mewe, R. 1978, A&AS, 32, 283
Grevesse, N., Asplund, M., & Sauval, A. J. 2007, Space Sci. Rev., 130, 105
Gu, M. F. 2003, ApJ, 590, 1131
Jelinsky, P., Vallerga, J.V., & Edelstein, J. 1995, ApJ, 441, 653
Kafatos, M. 1973, ApJ, 182, 433
Kahn, F. D. 1981, in Investigating the Universe, edited by F. D. Kahn, Reidel (Dordrecht), p. 1.
Kato, T. 1976, ApJS, 30, 397
Karas, J. M., & Latter, R. 1961, ApJS, 6, 167
Kingdon, J., & Ferland, G. J. 1996, ApJS, 106, 205
Koo, B.-C., & McKee, C. F. 1992, ApJ, 388, 93
Korpi, M. J., Brandenburg, A., Shukurov, A., Tuominen, I., & Nordlund, Å. 1999, ApJ, 514, L99
Korpi, M. J., Brandenburg, A., Shukurov, A., Tuominen, I. 1999b, A&A, 350, 230
Lestinsky, M., Badnell, N. R., Bernhardt, D., et al. 2009, ApJ, 698, 648
Lockman, F. J. 1984, ApJ, 283, 90
Lukic, D. V., Schnell, M., Savin, D. W., et al. 2005, ApJ, 664, 1244
McCann, D., Almy, R., Apodaca, E., Bergmann-Tiest, W., et al. 2002, ApJ, 576, 188
Mac Low, M.-M., McCray, R., & Norman, M. L. 1989, ApJ, 337, 141
Matsuki, C., Mazzetti, G., Finkenthal, M., Mazzotta, P., Fournier, K. B., Kaastra, J., & Puiatti, M. E., 2007, J. Phys. B: At. Mol. Opt. Phys., 40, 3569 (MAT2007)
Mazzotta, P., Mazzetti, G., Colafrancesco, S., & Vittorio, N., 1998, A&A, 333, 403 (MAZ1998)
McCray, R., & Kafatos, M. 1987, ApJ, 317, 190
McCammon, D., Almy, R., Apodaca, E., Bergmann-Tiest, W., & et al. 2002, ApJ, 576, 188
Mewe, R., Gronenschild, E. H. B. M., & van den Oord, G. H. J., 1985, A&AS, 62, 197
Mewe, R., Lemen, J. R., & van den Oord, G. H. J., 1986, A&AS, 65, 511
Mineshige, S., Shibata, K., & Shapiro, P. R. 1993, ApJ, 409, 663
Mitnik, D. M., & Badnell, N. R. 2004, A&A, 425, 1153
Norman, C. A., & Ikeuchi, S. 1989, ApJ, 345, 372
Orban, I., Böhm, S., Loch, S., & Schuch, R. 2008, A&A, 489, 829
Orban, I., Altun, Z., Källberg, A., & et al., 2009, A&A, 498, 909
Parker, E. N. 1966, ApJ, 145, 811
Penston, M. V. 1970, ApJ, 162, 771
Reynolds, R. J. 1985, ApJ, 294, 256
Rosen, A., Bregman, J. N., & Norman, M. L. 1993, ApJ, 413, 137
Bubbles, Superbubbles and Non-Equilibrium Ionization

Rosen, A., & Bregman, J. N. 1995, ApJ, 440, 634
Sanders, W. T., Edgar, R. J., Kraushaar, W. L., McCammon, D., & Morgenthaler, J. P. 2001, ApJ 554, 694
Savin, D. W., Gwinner, G., Grieser, M., et al. 2006, ApJ, 642, 1275
Schmidt, E. W., Schippers, S., Müller, A., et al. 2006, ApJ, 641, L157
Schmidt, E. W., Schippers, S., Bernhardt, D., et al. 2008, A&A, 492, 265
Schmutzler, T. & Tscharnuter, W. M. 1993, A&A, 273, 318
Shapiro, P. R., & Moore, R. T. 1976, ApJ, 207, 460
Spirko, J. A., Zirbel, J. J., & Hickman, A. P. 2003, J. Phys. B: At. Mol. Opt. Phys., 36, 1645
Stern, R., Wang, E., & Bowyer, S. 1978, ApJS, 37, 195
Stil, J., Wityk, N., Ouyed, R., & Taylor, A. R. 2009, ApJ, 701, 330
Sutherland, R. S., & Dopita, M. A. 1993, ApJS, 88, 253
Suno, H., & Kato, T. 2006, ADNDT, 92, 407
Tomisaka, K., & Ikeuchi, S., 1986, PASJ, 38, 697
Tomisaka, K. 1998, MNRAS 298, 797
Tucker, W. H., & Gould, R. J. 1966, ApJ, 144, 244
Trümper, J. 1983, Adv. Sp. Res. 2(4), 241
Verner, D. A., & Ferland, G. J., 1996, ApJS, 103, 467
Vogler, A., & Pietsch, W. 1996, A&A 311, 35
von Weizsäcker, C. F. 1951, ApJ 114, 165
Wang, J.G., Stancil, P. C., Rakovi´c, M. J., Schultz, D. R., & Zygelman, B. 2002, in NASA Laboratory Astrophysics Workshop, NASA/CP-2002-21186, p. 101.
Wang, J.G., Turner, A. R., Cooper, D. L., Schultz, D. R., Rakovi´c, M. J., Fritsch, W., Stancil, P. C., & Zygelman, B. 2002, J. Phys. B: At. Mol. Opt. Phys., 35, 3137
Wang, J.G., Stancil, P. C., Turner A. R., & Cooper, D. L. 2003, Phys. Rev. A, 67, 12710
Wang, J. G., He, B., Ning, Y., Liu, C. L., & Yan, J. 2006, Phys. Rev. A, 74, 52709
Wu, Y., Qi, Y. Y., Zou, S. Y., Wang, J. G., Li, Y., Buenker, R. J., & Stancil, P. C. 2009, Phys Rev A, 79, 62711
Zatsarinny, O., Gorczyca, T. W., Korista, K. T., Badnell, N. R., & Savin, D. W. 2003, A&A, 412, 587
Zatsarinny, O., Gorczyca, T. W., Korista, K. T., Badnell, N. R., & Savin, D. W. 2004, A&A, 417, 1173
Zatsarinny, O., Gorczyca, T. W., Fu, J., Korista, K. T., Badnell, N. R., & Savin, D. W. 2006, A&A, 447, 379
Zhao, L. B., Stancil, P. C., Gu, J. P., Liebermann, H.-P., Li, Y., Funke, P., Buenker, R. J., Zygelman, B., Kimura, M., & Dalgarno, A. 2004, ApJ, 615, 1063
Zhao, L. B., Stancil, P. C., Liebermann, H. P., Funke, P., & Buenker, R. J. 2005a, Phys Rev A, 71, 60701(R)
Zhao, L. B., Stancil, P. C., Gu, J.-P., Hirsch, G., Buenker, R. J., Imai, T. W., & Kimura, M. 2005b, Phys Rev A, 72, 32719
Zhao, L. B., Wang, J. C., Stancil, P. C., Gu, J. P., Liebermann, H.-P., Buenker, R. J., & Kimura, M., 2006, J. Phys. B: At. Mol. Opt. Phys., 39, 5151