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The Effects of Elemental Abundances on Fitting Supernova Remnant Models to Data

Denis A. Leahy

Department of Physics and Astronomy, University of Calgary, Calgary, AB T2N 1N4, Canada; leahy@ucalgary.ca

Abstract: Models for supernova remnant (SNR) evolution can be used to determine the energy of the explosion, the age of the SNR, and the density of the surrounding medium by matching observations. Observed SNR properties derived from the X-ray spectrum include the electron temperature (kT_e) and emission measure (EM) of the shocked gas. SNR models are based on hydrodynamic solutions for density, pressure, and velocity. The relations between these and kT_e or EM depend on the three inputs of composition, ionization state, and electron-ion temperature ratio (T_e/T_I). The standard definitions and the XSPEC definitions for kT_e and EM have important differences that are not well-known. The same definition used by observers of SNRs must be used in models for correct interpretation. Here, the effects of the three inputs on standard and on XSPEC versions of kT_e and EM are investigated, with examples. The ratio of standard EM to the XSPEC value ranges widely, between $\sim 10^{-3}$ to ~ 1, with smallest ratios for gas with low hydrogen abundance. The standard kT_e differs from the XSPEC value by less than a few percent. For the illustrative example SNR J0049-7314, the ejecta component is shown to be consistent with core-collapse composition and a stellar wind environment.

Keywords: supernova remnants; supernova energetics; interstellar medium density

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1. Introduction

Supernova remnants (SNRs) are a significant force in galaxies: they add energy to the interstellar medium (ISM) (e.g., [1]) and spread elements, which are created in the supernovae (SN) explosion around the ISM (e.g., [2]). From SNR studies we can learn about the end states of stellar evolution, the properties of ISM, and the impact of SN explosions on the Galaxy. SNR research has several purposes, including learning about SN explosions and the effects of SN mass and energy input to the ISM. Research on the mechanism of SN explosions has made great advances in recent years (e.g., [3] and references therein).

The observational data for a given SNR depends on the brightness of emissions in different wavebands and by the instruments used for the observations. SNRs in our Galaxy have been mainly discovered by their radio emission [4]. To characterize a SNR, which has most of its energy contained in the X-ray emitting shocked gas, X-ray spectral observations are required. In the past two decades, X-ray observational capabilities have increased dramatically in spatial and spectral resolution and in sensitivity. The highest spatial resolution is available with Chandra, allowing spatially resolved studies of small angular size SNRs such as G21.5-09 [5] and 1E0102.2-7219 [6]. High sensitivity observations are exemplied by those with XMM-Newton, e.g., detection of a recombining plasma in W44 [7] and with Suzaku, e.g., detection of spatially variable electron temperature and asymmetric ejecta in SNR CTB 1 [8].

Among the early important theoretical studies of X-ray spectra emitted by SNRs is that of [9]. The X-ray spectrum diagnoses the amount of shocked gas, via the emission measure (EM), and the shocked gas electron temperature (kT_e). X-ray observations of some historical SNR were modelled with tailored hydrodynamic simulations (e.g., [10]). For Type Ia explosions, spherically symmetric (1-dimensional) models have been applied to understand bulk SNR properties [11] with a numerical code that includes the coupling between hydrodynamics and nuclear reactions [12]. For core-collapse (CC) SN the simulations have advanced to include three dimensions (3D) and are able to fit observed emission line velocities in cases where the observations are good enough, such as SN1987A [13] and Cas A [14]. SN 1987A is of particular interest because it exhibits a clear 3D structure and requires simulations with 3D complexity to be understood, including the possibility of a binary merger progenitor [15].

The majority of Galactic SNRs have less complete observations than the historical SNRs, including no observed ages. For these, usually a basic Sedov model with assumed energy and ISM density was applied to obtain age estimates. However, SNRs have a wide range of energies and ISM densities ([16–19]), which were obtained using more physically realistic models than the Sedov model. Some dispersion in energy is expected based on simulations of core-collapse (CC) SN ([20], and references therein). As discussed by the comparison of simulations with observations of CC SN energies [21], both are heavily biased, implying our knowledge of SN energies is still quite incomplete.

To characterize SNRs, we developed a set of models which are based on hydrodynamic calculations with scalings derived using the unified model of [22]. These models assume spherical symmetry and are described in [23,24]. They also assumed standard definitions of EM and kT_e. The observed quantities of electron temperatures and emission measures of the hot plasma, for forward-shocked and for reverse-shocked gas are calculated in the model. These models are important to enable the process of using X-ray observations, normally analyzed using XSPEC [25] to determine EM and kT_e, to obtain the physical properties of a SNR, such as explosion energy, age, and ISM density.

This work includes a detailed consideration of the effect of composition and partial ionization on the emission measures and shock temperatures, for both standard and XSPEC definitions, that are calculated using hydrodynamic simulations. This is an important extension of the models presented in [23] and will allow model users to choose the same definitions as used by observers. In Section 2.1, we present an overview of the SNR model. In Section 2.2, the standard and XSPEC definitions of emission measure (EM) and EM-weighted gas temperature (kT_{EM}) are compared and related to mean molecular weights. In Section 2.3.1, the relation of gas temperature to electron temperature ($kT_{e,EM}$) is discussed. In Section 2.3, the dependence of temperature and emission measure of shocked gas on chemical composition and ionization state are determined. In Sections 3.2 and 3.3, the scaling relations for EM and $kT_{e,EM}$ on mean molecular weights are given. An example application is given in Section 3.4 and considerations of input from other wavelengths than X-ray are briefly discussed in Section 3.5. The conclusions are summarized in Section 4.

2. Analysis

The assumption here is that a hydrodynamic model for SNR evolution is calculated, with fundamental variables of density, pressure and velocity of the gas. The aim of that model is to reproduce observed quantities of a given SNR, in particular EM and $kT_{e,EM}$, by relating the computed hydrodynamic variables to the observed variables. To make simplifying assumptions in the calculations of effects of chemical composition and ionization of the gas, a reference model is chosen. This is the spherically symmetric model of [23] (and references therein). However, the results below apply to any SNR model subject to the particular assumptions made by that model.

2.1. The Model for SNR Evolution

A SNR is the interaction of the SN ejecta with the interstellar medium (ISM). The various stages of evolution of a SNR are labelled the ejecta-dominated stage (ED), the adiabatic or Sedov-Taylor stage (ST), the radiative pressure-driven snowplow (PDS) and the radiative momentum-conserving shell (MCS). These stages are reviewed in, e.g., [4,22,24,26,27]. In addition, there are the transitions between stages, called ED to ST, ST to PDS, and PDS to

MCS, respectively. The ED to ST stage is important because the SNR is still bright, and it is long-lived enough [23] that a significant fraction of SNRs are likely in this phase.

For simplicity, our models assume that the SN ejecta and ISM are spherically symmetric. The ISM density profile is a power-law centered on the SN explosion, given by $\rho_{ISM} = \rho_s r^{-s}$, with s = 0 (constant density medium) or s = 2 (stellar wind density profile). The unshocked ejecta has a power-law density $\rho_{ej} \propto r^{-n}$ envelope with constant density core. With these profiles, the ED phase of the SNR evolution has a self-similar evolution [28,29] prior to the reverse shock hitting the core [22]. The evolution of SNR shock radius was extended for the ED to ST and ST phases by [22].

The model for SNR evolution that we use is partly based on the TM99 analytic solutions, with additional features. A detailed description of the model is given in [23]. Hydrodynamic variables for the interior structure of the SNR are calculated from hydrodynamic simulations which cover ED, ED to ST, and ST phases. The scaling relations of the unified solution of [22] are used to keep the size of grid of hydro models feasible for calculation. Electron-ion temperature equilibration (T_e/T_I) is included after the hydro calculations. T_e/T_I is calculated using the Coulomb collisional electron heating mechanism, consistent with the observational results of [30]. The emission measure (EM) and emission measure-weighted electron temperature ($T_{e,EM}$) are calculated from the hydrodynamic variables, gas composition, and T_e/T_I. The inverse modelling problem was solved by [17]. This takes as input the SNR observed properties and determines the initial properties of the SNR.

The current version of the SNR modelling program calculates EM and $kT_{e,EM}$ using the standard definition of these quantities. This work presents the full dependence of EM and $kT_{e,EM}$ on composition, ionization, and T_e/T_I. It extends the calculations to include the definitions of EM and $kT_{e,EM}$ used by the standard X-ray spectrum modelling program XSPEC, which differ in important ways from the standard definitions (see Section 2.2 below). This extension is essential to allow users of the model to choose the same definition used by observers in deriving $\boldsymbol{EM}$ and $\boldsymbol{kT_e}$ from the X-rays spectrum, so that the interpretation of SNR properties is correct.

2.2. Emission Measure (EM) and EM-Weighted Gas Temperature (kT_{EM})

Observed SNR quantities from the X-ray spectrum to be modelled are the emission measure, EM, and the EM-weighted electron temperature, $kT_{e,EM}$, for both forward-shocked ISM (FS) and reverse-shocked ejecta (RS). The relation between $kT_{e,EM}$ and gas temperature kT_{EM} is discussed in Section 2.3.1 below. The standard definition of EM is:

$$EM = \int n_e(r) n_H(r) dV \tag{1}$$

with n_e and n_H the number densities of electrons and hydrogen nuclei, respectively, and the integration is over the volume of the emitting gas. kT_{EM} is given by

$$kT_{EM} = \int n_e(r) n_H(r) kT(r) dV / EM \tag{2}$$

However, the EM used by XSPEC and by observers, called EM_{XS} here, has a modified definition of n_H [31], called $n_{H,XS}$ here, designed to include cases of very low hydrogen abundance without diverging. The total ion density n_I is converted to $n_{H,XS}$ using cosmic abundances: $n_{H,XS} = n_I \frac{x_{H,C}}{\sum_j x_{j,C}} = n_I x_{H,C}$, where $x_{j,C}$ are number fractions of all elements for cosmic abundances and the latter expression assumes they are normalized ($\sum_j x_{j,C} = 1$). Thus, one has

$$EM_{XS} = \int n_e(r) n_{H,XS}(r) dV = x_{H,C} \int n_e(r) n_I(r) dV \tag{3}$$

with $x_{H,C} = 0.921$[1] the fractional number abundance of H. EM_{XS} defined in terms of the ion density whereas EM is defined in terms of hydrogen density. $kT_{EM,XS}$ is found using EM_{XS}:

$$kT_{EM,XS} = \int n_e(r) n_{H,XS}(r) kT(r) dV / EM_{XS} \tag{4}$$

If $n_I(r) \propto n_H(r)$ then one has $kT_{EM,XS} = kT_{EM}$. In general, spatial variations in composition violate a constant proportionality, so $kT_{EM,XS}$ and kT_{EM} are different.

2.3. Dependence of EM and kT_{EM} on Mean Molecular Weights and Ionization

A hydrodynamic simulation of a SNR yields the variables of mass density, pressure and velocity. To convert to gas temperature $T(r)$, total number density n, hydrogen number density $n_H(r)$, ion number density $n_I(r)$, and electron number density $n_e(r)$ needed for EM and kT_{EM}, one uses the definition of the molecular weights (μs),

$$\rho = \mu m_H n = \mu_H m_H n_H = \mu_I m_H n_I = \mu_e m_H n_e \tag{5}$$

Temperature is determined using the ideal gas law,

$$T = \frac{\mu m_H}{k_B} \frac{P}{\rho} \tag{6}$$

The dependence on ionization state of the gas is included in the μs.

EM and kT_{EM} for FS and RS gas in terms of mass density and pressure are:

$$\begin{aligned}
EM_{FS} &= \int_{R_{CD}}^{R_{FS}} \frac{\rho(r)^2}{m_H^2 \mu_{e,FS}(r) \mu_{H,FS}(r)} dV \\
&= \frac{1}{\mu_{e,FS} \mu_{H,FS} m_H^2} \int_{R_{CD}}^{R_{FS}} \rho(r)^2 / dV \\
EM_{RS} &= \int_{R_{RS}}^{R_{CD}} \frac{\rho(r)^2}{m_H^2 \mu_{e,RS}(r) \mu_{H,RS}(r)} dV \\
&= \frac{1}{\mu_{e,RS} \mu_{H,RS} m_H^2} \int_{R_{RS}}^{R_{CD}} \rho(r)^2 dV
\end{aligned} \tag{7}$$

$$\begin{aligned}
kT_{EM,FS} &= \int_{R_{CD}}^{R_{FS}} \frac{\rho(r)^2}{m_H^2 \mu_{e,FS}(r) \mu_{H,FS}(r)} \frac{P(r) \mu_{FS}(r) m_H}{\rho(r) k_B} dV / EM_{FS} \\
&= \frac{\mu_{FS} m_H}{k_B} \int_{R_{CD}}^{R_{FS}} \rho(r) P(r) dV / \int_{R_{CD}}^{R_{FS}} \rho(r)^2 dV \\
kT_{EM,RS} &= \int_{R_{RS}}^{R_{CD}} \frac{\rho(r)^2}{m_H^2 \mu_{e,RS}(r) \mu_{H,RS}(r)} \frac{P(r) \mu_{RS}(r) m_H}{\rho(r) k_B} dV / EM_{RS} \\
&= \frac{\mu_{RS} m_H}{k_B} \int_{R_{RS}}^{R_{CD}} \rho(r) P(r) dV / \int_{R_{RS}}^{R_{CD}} \rho(r)^2 dV
\end{aligned} \tag{8}$$

where the μs are assumed spatially uniform to simplify the integrals[2]. For EM_{RS} and $kT_{EM,RS}$ the lower limit of integration is 0 after the RS reaches the center of the SNR.

For XSPEC-defined quantities, one has:

$$\begin{aligned}
EM_{XS,FS} &= x_{H,C} \int_{R_{CD}}^{R_{FS}} \rho(r)^2 / (m_H^2 \mu_{e,FS}(r) \mu_{I,FS}(r)) dV \\
&= \frac{x_{H,C}}{\mu_{e,FS} \mu_{I,FS} m_H^2} \int_{R_{CD}}^{R_{FS}} \rho(r)^2 dV \\
EM_{XS,RS} &= x_{H,C} \int_{R_{RS}}^{R_{CD}} \rho(r)^2 / (m_H^2 \mu_{e,RS}(r) \mu_{I,RS}(r)) dV \\
&= \frac{x_{H,C}}{\mu_{e,RS} \mu_{I,RS} m_H^2} \int_{R_{RS}}^{R_{CD}} \rho(r)^2 dV
\end{aligned} \tag{9}$$

$$\begin{aligned} kT_{EM,XS,FS} &= \int_{R_{CD}}^{R_{FS}} \frac{\rho(r)^2 x_{H,C}}{m_H^2 \mu_{e,FS}(r)\mu_{I,FS}(r)} \frac{P(r)\mu_{FS}(r)m_H}{\rho k_B} dV / EM_{XS,FS} \\ &= \frac{\mu_{FS} m_H}{k_B} \int_{R_{CD}}^{R_{FS}} \rho(r)P(r)dV / \int_{R_{CD}}^{R_{FS}} \rho(r)^2 dV \\ kT_{EM,XS,RS} &= \int_{R_{RS}}^{R_{CD}} \frac{\rho(r)^2 x_{H,C}}{m_H^2 \mu_{e,RS}(r)\mu_{I,RS}(r)} \frac{P(r)\mu_{RS}(r)m_H}{\rho k_B} dV / EM_{XS,RS} \\ &= \frac{\mu_{RS} m_H}{k_B} \int_{R_{RS}}^{R_{CD}} \rho(r)P(r)dV / \int_{R_{RS}}^{R_{CD}} \rho(r)^2 dV \end{aligned} \quad (10)$$

where the μs are assumed spatially uniform to simplify the integrals.

2.3.1. Electron Temperature and Electron-Ion Equilibration

The EM-weighted electron temperature, T_e, is measured by the X-ray spectrum. The relation between gas T, electron T_e and ion T_I, from $P = P_e + P_I$, is:

$$T/\mu = T_e/\mu_e + T_I/\mu_I \quad (11)$$

In general, the spatial dependence of $T(r)$, $T_e(r)$ and $T_I(r)$ is complex.

In the case that shocked SNR gas has T_e and T_I equilibrated by Coulomb collisions [33] and is not old enough to have radiative losses, the electron-to-ion temperature ratio $g(t) = T_e(t)/T_I(t) = g(T_s(t), T_e(t), t)$ increases to unity with t the age of a given parcel of gas since it was shocked. The calculation of g is summarized in [24].

$T_{e,FS}(r)$ and $T_{e,RS}(r)$ are found using Equations (6) and (11) which give $T_e = \frac{1}{1/\mu e + 1/(g\mu_I)} \frac{T}{\mu}$:

$$\begin{aligned} T_{e,FS}(r) &= f_{T,FS}(r) \frac{P(r)m_H}{\rho(r)k_B} \\ T_{e,RS}(r) &= f_{T,RS}(r) \frac{P(r)m_H}{\rho(r)k_B} \end{aligned} \quad (12)$$

with $f_{T,FS}(r) = \frac{1}{1/\mu_{e,FS}(r) + g(r)/\mu_{I,FS}(r)}$ and $f_{T,RS}(r) = \frac{1}{1/\mu_{e,RS}(r) + g(r)/\mu_{I,RS}(r)}$. $f_{T,FS}$ and $f_{T,RS}$ are constants in the approximations of uniform μs and uniform g_{FS} and g_{RS}.

The standard FS and RS EM-weighted electron temperatures are the same as those given by Equation (8) except for inclusion of extra factors $f_{T,FS}(r)/\mu_{FS}(r)$ and $f_{T,RS}(r)/\mu_{RS}(r)$ in the integrals for $kT_{e,EM,FS}$ and $kT_{e,EM,RS}$. The XSPEC-defined FS and RS EM-weighted electron temperatures are:

$$\begin{aligned} kT_{e,EM,XS,FS} &= \int_{R_{CD}}^{R_{FS}} \frac{\rho(r)^2 x_{H,C}}{m_H^2 \mu_{e,FS}(r)\mu_{I,FS}(r)} \frac{f_{T,FS}(r)P(r)m_H}{\rho(r) k_B} dV / EM_{XS,FS} \\ &= \frac{f_{T,FS} m_H}{k_B} \int_{R_{CD}}^{R_{FS}} \rho(r)P(r)dV / \int_{R_{CD}}^{R_{FS}} \rho(r)^2 dV \\ kT_{e,EM,XS,RS} &= \int_{R_{RS}}^{R_{CD}} \frac{\rho(r)^2 x_{H,C}}{m_H^2 \mu_{e,RS}(r)\mu_{I,RS}(r)} \frac{f_{T,RS}(r)P(r)m_H}{\rho(r) k_B} dV / EM_{XS,RS} \\ &= \frac{f_{T,RS} m_H}{k_B} \int_{R_{RS}}^{R_{CD}} \rho(r)P(r)dV / \int_{R_{RS}}^{R_{CD}} \rho(r)^2 dV \end{aligned} \quad (13)$$

where the second expressions for $kT_{e,EM,XS,FS}$ and $kT_{e,EM,XS,RS}$ apply in the case of uniform μs and gs. In that case, the standard and the XSPEC versions are identical[3]:

$$\begin{aligned} kT_{e,EM,XS,FS} &= kT_{e,EM,FS} \\ kT_{e,EM,XS,RS} &= kT_{e,EM,RS} \end{aligned} \quad (14)$$

3. Results and Discussion

3.1. Definition of EM

The standard EM is defined in terms of hydrogen density, whereas EM_{XS} is defined in terms of the ion density then converted to an equivalent hydroden normalization (Equation (9)). $kT_{e,EM}$ is weighted by $n_e n_H$ whereas $kT_{e,EM,XS}$ is weighted by $n_e n_I$. The measured kT is best estimated by weighting $kT_e(r)$ by the X-ray emissivity integrated over the emission volume. In the case of high hydrogen abundance $kT_{e,EM}$ and $kT_{e,EM,XS}$ are nearly the same, but for low hydrogen abundance, X-ray emissivity is closer to proportional to $n_e n_I$ than to $n_e n_H$. Thus, $kT_{e,EM,XS}$ is the better measure. Overall, for properties measured using the X-ray spectrum, sensitive to all electrons and ions, the XSPEC definitions of EM and kT_e are better, despite the artifact that it is labelled with n_H rather than n_I.

3.2. Scaling Relations for EM and kT_{EM}

For simplicity, spatially uniform $\mu_{e,FS}$, $\mu_{I,FS}$, $\mu_{H,FS}$, $\mu_{e,RS}$, $\mu_{I,RS}$, $\mu_{H,RS}$, g_{FS} and g_{RS} are assumed[4]. EM and $kT_{e,EM}$ are compared between two sets of μs and gs, labelled set A and set B, using the equations above:

$$\begin{aligned}
EM_{FS,B} \times \mu_{e,FS,B}\mu_{H,FS,B} &= EM_{FS,A} \times \mu_{e,FS,A}\mu_{H,FS,A} \\
EM_{RS,B} \times \mu_{e,RS,B}\mu_{H,RS,B} &= EM_{RS,A} \times \mu_{e,RS,A}\mu_{H,RS,A} \\
EM_{FS,XS,B} \times \mu_{e,FS,B}\mu_{I,FS,B} &= EM_{FS,XS,A} \times \mu_{e,FS,A}\mu_{I,FS,A} \\
EM_{RS,XS,B} \times \mu_{e,RS,B}\mu_{I,RS,B} &= EM_{RS,XS,A} \times \mu_{e,RS,A}\mu_{I,RS,A} \\
kT_{e,EM,FS,B}/f_{T,FS,B} &= kT_{e,EM,FS,A}/f_{T,FS,A} \\
kT_{e,EM,RS,B}/f_{T,RS,B} &= kT_{e,EM,RS,A}/f_{T,RS,A}
\end{aligned} \tag{15}$$

The standard and XSPEC values of EM are related by:

$$\begin{aligned}
EM_{FS,XS} \times \mu_{I,FS}/x_{H,C} &= EM_{FS} \times \mu_{H,FS} \\
EM_{RS,XS} \times \mu_{I,RS}/x_{H,C} &= EM_{RS} \times \mu_{H,RS}
\end{aligned} \tag{16}$$

For the case that $g_{RS,A}$ and $g_{RS,B}$ are the same,

$$kT_{e,EM,RS,B}\left(\frac{1}{\mu_{e,RS,B}} + \frac{g_{RS}}{\mu_{I,RS,B}}\right) = kT_{e,EM,RS,A}\left(\frac{1}{\mu_{e,RS,A}} + \frac{g_{RS}}{\mu_{I,RS,A}}\right) \tag{17}$$

For older SNRs, one has $g_{RS,A} = g_{RS,B} = 1$, which gives:

$$kT_{e,EM,RS,B}/\mu_{RS,B} = kT_{e,EM,RS,A}/\mu_{RS,A} \tag{18}$$

For young SNRs (age less than a few hundred years) $g_{2,A} << 1$ and $g_{2,B} << 1$, one has:

$$kT_{e,EM,RS,B}/\mu_{e,RS,B} = kT_{e,EM,RS,A}/\mu_{e,RS,A} \tag{19}$$

3.3. Chemical Composition and Partial Ionization Examples

Table 1 lists μs for different ISM/FS and ejecta/RS compositions and different ionization levels. The μs for FS (first two rows) have very little variation ($\sim$1%) with composition. Thus, $kT_{e,EM,FS}$, EM_{FS} and $EM_{FS,XS}$ show very little variation with composition, less than typical errors in measured EM and kT_e. For solar composition EM_{FS} and $EM_{FS,XS}$ are the same: $\mu_{I,FS}/x_{H,C} = \mu_{H,FS} = 1.356$.

Table 1. Summary of Mean Molecular Weights.

Composition	μ_H	μ_e [1]	μ_e [2]	μ_e^c [3]	μ_I	μ^a [1]	μ^b [2]	μ^c [3]
Solar [4]	1.356	1.151	2.303	1.250	1.250	0.599	0.810	0.625
SMC [5]	1.340	1.145	2.290	1.236	1.236	0.594	0.803	0.618
CC-type ejecta [5]	1.810	1.289	2.578	1.542	1.542	0.702	0.965	0.771
Type Ia ejecta [6]	1327	2.093	4.187	35.57	35.57	1.977	3.746	17.78
Mixture 1 CC-Ia [7]	12.24	1.894	3.789	7.789	7.789	1.524	2.549	3.894
Mixture 2 CC-Ia [8]	3.615	1.596	3.191	2.956	2.956	1.036	1.535	1.478
Mixture ISM-CC [9]	1.551	1.216	2.433	1.381	1.381	0.647	0.881	0.690
Mixture ISM-Ia [10]	2.710	1.486	2.971	2.415	2.415	0.920	1.332	1.207
Pure oxygen	∞	2.000	4.000	16.00	16.00	1.778	3.200	8.000
Pure iron	∞	2.154	4.308	56.00	56.00	2.074	4.000	28.00

[1] Fully ionized plasma. [2] Each element 50% ionized. [3] Each element singly ionized. [4] Abundances from [32]. [5] Abundances from [34]. [6] Abundances from [23]. [7] Geometric mean of CC-type and Type Ia abundances. [8] Equal mass mixture of CC-type and Type Ia abundances. [9] Equal mass mixture of Solar and CC-type abundances. [10] Equal mass mixture of Solar and Type Ia abundances.

For RS/ejecta gas, the μs can vary widely as shown in rows 3–10 of Table 1. The standard to XSPEC EM ratio $\frac{EM_{RS}}{EM_{RS,XS}}$ varies from 0 (cases of no H in the ejecta), to 0.029 (for the adopted Type Ia abundances), to values near 1 for cases with significant H abundance (including the adopted CC-type and ISM-CC mixture) As noted earlier the XSPEC definition is superior. In particular, when the H abundance is 0 the standard EM is 0 and completely fails to represent the emission from the gas.

The effect of changing μs on EM_{XS} of RS gas is shown by the ratios of $\frac{EM_{RS,XS,B}}{EM_{RS,XS,A}}$, with A = solar abundances. Table 2 gives this for two cases of ionization (last two columns): fully ionized plasma and singly ionized plasma. The composition for the fully ionized case results in a ratio ranging from 0.012 for pure Fe (smaller EM for pure Fe) to 1.017 (SMC abundances with more H than solar). For the singly ionized case, the ratio ranges from $\sim 5 \times 10^{-4}$ to 1.023 (SMC abundances). To obtain $\frac{EM_{RS,XS,B}}{EM_{RS,XS,A}}$ for A different from solar, one divides the ratio of B to solar to that for A to solar. e.g., $\frac{EM_{RS,XS,B=Ia}}{EM_{RS,XS,A=CC}}$, fully ionized, is 0.0267 and $\frac{EM_{RS,XS,B=PureFe}}{EM_{RS,XS,A=Ia}}$, fully ionized, is 0.617.

Table 2. Emission Measure Ratios.

Composition [1]	$\frac{EM_{RS}}{EM_{RS,XS}}$	$\frac{EM_{RS,XS,B}}{EM_{RS,XS,\odot}}$ [2]	$\frac{EM_{RS,XS,B}}{EM_{RS,XS,\odot}}$ [3]
Solar	1	1	1
SMC	1.001	1.017	1.023
CC-type ejecta	0.925	0.724	0.657
Type Ia ejecta	0.0291	0.0193	1.24×10^{-3}
Mixture 1 CC-Ia	0.691	0.0975	0.0258
Mixture 2 CC-Ia	0.888	0.305	0.179
Mixture ISM-CC	0.967	0.857	0.820
Mixture ISM-Ia	0.968	0.401	0.268
Pure oxygen	0	0.0450	6.10×10^{-3}
Pure iron	0	0.0119	4.98×10^{-4}

[1] See Table 1 for composition notes. [2] Case ⊙ is solar, Case B is from Composition row. Fully ionized and 50% ionized give the same ratio. [3] Case ⊙ is solar, Case B is from Composition row. Each element 50% ionized.

The H and heavy element abundances in Type Ia or CC-type could be different than assumed. As test cases, μs are shown for two mixtures of CC-type and Ia-type ejecta: a geometric mean, and an equal mass mixture. The equal mass mixture has more H, resulting in significantly lower μs.

The effect of partial ionization is illustrated in Table 1. Only μ_e and μ are affected. The ratio of μ_e for singly ionized plasma to μ_e for fully ionized ranges from 1.08 (SMC) to 26.0

(pure Fe). 50% ionized plasma has μ_e larger than for fully ionized by a factor of 2, whereas μ_e can be higher (cases with high H) or lower (cases with low H) than μ_e for singly ionized.

The effect of ionization on μ is smaller than for μ_e, with ratio of μ (singly ionized) to μ (fully ionized) ranging from 1.04 (SMC) to 13.5 (pure Fe). 50% ionized plasma has μ larger than for fully ionized by a factor of 1.35 (SMC) to 1.93 (pure Fe), whereas μ can be higher (cases with high H) or lower (cases with low H) than μ for singly ionized.

kT_e depends on the μs, as follows. For older SNRs ($g = 1$) Equation (18) shows that RS temperatures for fully ionized gas can be larger than for solar composition up to a factor of 3.46 (pure Fe) or smaller by a factor of 0.99 (SMC abundances). In the extreme case of singly ionized gas, T_e can be larger than for solar composition up to a factor of 44.8 (pure Fe) or smaller by a factor of 0.99 (SMC abundances). For very young SNRs ($g << 1$) Equation (19) applies, yielding smaller changes than for the fully ionized case: $kT_{e,EM,RS,B}/kT_{e,EM,RS,\odot}$ varies from 0.995 (for SMC) to 1.87 (pure Fe). For singly ionized gas, $kT_{e,EM,RS,B}/kT_{e,EM,RS,\odot}$ has the same range as for SNRs with $g = 1$: 0.995 to 44.8. Shock temperatures in SNRs are generally high enough that the gas is ∼50% or more ionized, so the ratios are less extreme than for the singly ionized case. In general, more heavy elements in the ejecta make the RS temperature higher.

3.4. Example Application to a SNR with Reverse Shock Measured

As described above, the differences between standard and XSPEC values of kT_e and EM are largest for the RS and for cases with low H abundance in the ejecta. We illustrate the difference for an observed SNR using one with RS measured from the Small Magellanic Cloud: SNR J0049-7314 and for two cases of composition: CC and Ia. The measured kT_e's and EMs are from [35] and were compared to SNR models by [16]. We take the CC and Ia compositions adopted by [24].

The measured $kT_{e,FS}$ and EM_{FS} for SNR J0049-7314 modelled by [16] assumed CC composition and standard definitions of kT_e and EM. However, the observed values were derived using XSPEC definitions. Our models assume uniform composition ISM and uniform composition ejecta, so that the standard and XSPEC values of $kT_{e,FS}$ are the same (both use SMC composition). However, $kT_{e,RS}$ depends on composition as specified by Equation (17). The age of SNR J0049-7314 is ∼18,000 yr if in a uniform ISM, or ∼2000–6000 yr if in a stellar wind. Thus, it is old enough that we set the electron-ion temperature ratio close to 1. Then one obtains $kT_{e,RS,Ia} = 2.82 \times kT_{e,RS,CC}$. For EM_{RS}, we first obtain the relation between the normal and XSPEC RS values using Equation (16), which yields $EM_{RS,XS,CC} = 1.27 \times EM_{RS,CC}$. The relation between XSPEC values for CC and for Ia is given by the fourth line of Equation (15), which yields $EM_{RS,XS,Ia} = 2.67 \times 10^{-2}\ EM_{RS,XS,CC}$. The resulting model values of $kT_{e,RS}$ and $EM_{RS,XS}$ for the four cases s = 0 and 2 and n= 7 and 10 are given in Table 3.

Now we can assess the success of the various models. $EM_{RS,XS}$ is most sensitive to s, n and composition, so that is considered first. All Ia composition models yield too small $EM_{RS,XS}$, implying this is a CC SNR. All s = 0 models predict too small $EM_{RS,XS}$. The observed $EM_{RS,XS}$ is between model values for CC composition for (s, n) = (2, 7) and (2, 10). However the model $kT_{e,RS}$ is below the observed one: by factor 0.60 for (s, n) = (2, 7). Because $kT_{e,RS}$ and $EM_{RS,XS}$ depend in different ways on the μs, it is likely that adjustment of the composition could bring the model values into agreement with the observed ones within the uncertainties.

Table 3. SNR J0049-7314: CC and Ia reverse shock models [1].

	s, n	Composition [2]	$kT_{e,RS}$ (+, −) (keV)	$EM_{RS,XS}$ (+, −) (10^{56} cm^{-3})
Observed:		n/a	0.91 (+0.03, −0.03)	728 (+125, −99)
Models:	0.7	CC	3.6 (+1.1, −1.0)	0.14 (+0.03, −0.03)
	0.7	Ia	10.1 (+3.1, −2.8)	0.0037 (+0.0007, −0.0007)
	0.10	CC	2.2 (+0.6, −0.6)	0.24 (+0.04, −0.04)
	0.10	Ia	6.2 (+1.7, −1.7)	0.0065 (+0.0010, −0.0010)
	2.7	CC	0.55 (+0.16, −0.15)	130 (+149, −68)
	2.7	Ia	1.55 (+0.45, −0.42)	3.5 (+4.0, −1.8)
	2.10	CC	0.11 (+0.03, −0.03)	1660 (+1900, −890)
	2.10	Ia	0.31 (+0.08, −0.08)	44 (+51, −24)

[1] These are calculated by fitting the observed forward shock $kT_{e,EM,FS}$ and EM_{FS}. [2] CC and Ia μs are from Table 1.

3.5. Considerations from Other Wavelengths Than X-ray

The age, explosion energy, and ISM density are determined by the measured kT_e and EM of the forward shock from the X-ray spectrum. The FS radius is required and can come from any waveband, but normally the FS is bright in radio and X-ray, sometimes in optical or infrared. Additional constraints may be available such as expansion velocity for part or all of the SNR measured using proper motions determined by optical images [36] or from X-ray or radio images [37]. If available, this can be used to determine if the SNR is approximately symmetric by comparing with the predicted velocity from the spherically symmetric model. If not, then asymmetries should be modelled with more complex model calculations [13]. Infrared emission is sensitive to the dust content in SNR, which is formed in the ejecta and can give information on the composition and density of the SN ejecta [38].

4. Summary and Conclusions

The X-ray emission from a supernova remnant (SNR) is a powerful diagnostic of the state of the shocked plasma. Observed properties are shock radius, electron temperature (kT_e), and emission measure (EM) for forward-shocked (FS) and in some cases for reverse-shocked (RS) gas. Given a model, observations of FS gas can be used to determine the energy of the explosion, the age of the SNR, and the density of the surrounding medium. If RS gas emission is also detected, more properties of the SNR can be deduced [17] such as whether the SNR exploded in a uniform or stellar wind environment, and the range of allowable elemental compositions.

SNR models are based on hydrodynamic solutions for the fluid variables density, pressure and velocity. To calculate $\boldsymbol{EM_{FS}}$, $\boldsymbol{T_{e,FS}}$, $\boldsymbol{EM_{RS}}$ and $\boldsymbol{T_{e,RS}}$ from the hydrodynamic solutions, the values of FS molecular weights ($\boldsymbol{\mu_{FS}}$, $\boldsymbol{\mu_{e,FS}}$, $\boldsymbol{\mu_{I,FS}}$, $\boldsymbol{\mu_{H,FS}}$) and electron-to-ion temperature ratio ($\boldsymbol{g_{FS} = T_{e,FS}/T_{I,FS}}$) are required, and similar quantities for the $\boldsymbol{RS}$. The effects of composition, ionization and $\boldsymbol{g}$s on model-derived $\boldsymbol{kT_e}$ and $\boldsymbol{EM}$ and thus on derived SNR properties were investigated here.

The standard definitions and the XSPEC definitions for $\boldsymbol{kT_e}$ and $\boldsymbol{EM}$ have important differences that are not well-known. The standard definition of $\boldsymbol{EM}$ depends on H density whereas the XSPEC one depends on total ion density. The XSPEC definition is less sensitive to changes in hydrogen abundance, which is often poorly determined, so it is normally preferable to the standard definition. More importantly, modellers must use the same definition used by observers of SNRs for correct interpretation.

This work presents the dependence of $\boldsymbol{EM}$ and $\boldsymbol{kT_{e,EM}}$ on composition, ionization, and $\boldsymbol{T_e/T_I}$ for both standard and XSPEC definitions. Generally, $\boldsymbol{FS}$ gas has high H abundance, so the $\boldsymbol{\mu}$s do not depend strongly on composition and ionization. However, for the H-poor compositions of $\boldsymbol{RS}$ gas there are large variations in the $\boldsymbol{\mu}$s and $\boldsymbol{EM}$ values. The ratio of standard $\boldsymbol{EM}$ to the XSPEC value ranges widely, between $\sim 10^{-3}$ and ~ 1, with the smallest ratios for gas with low hydrogen abundance, such as the ejecta for Type Ia explosions. The formulas for $\boldsymbol{EM}$ and $\boldsymbol{kT_{e,EM}}$ simplify in the case of spatially uniform $\boldsymbol{\mu}$s and $\boldsymbol{g}$s. In this case, the standard and XSPEC definitions for kT_e are the same but those for EM are different, as summarized in Table 2.

The effects of electron-to-ion temperature ratio g on kT_e were shown to be composition dependent. For fully ionized and old gas, with $g = 1$, $kT_{e,RS}/kT_{e,RS,\odot}$ varies from $\simeq$1 (for H-rich compositions) to 3.46 (pure Fe), and for the extreme case of singly ionized gas $kT_{e,RS}/kT_{e,RS,\odot}$ varies from $\simeq$1 to 44.8. For young shocked gas, with $g << 1$, $kT_{e,RS}/kT_{e,RS,\odot}$ varies from $\simeq$1 to 1.87 for fully ionized gas, but the same range as for $g = 1$ for singly ionized gas.

The use of XSPEC definitions for EM and kT_e was illustrated for SNR J0049-7314, for which shocked FS gas and RS gas are observed. Only a small subset of the different SNR models are consistent with the observations, allowing determination of the external environment as a stellar wind, and showing allowable compositions of the ejecta contain significant H, consistent with core-collape origin.

Distances to Galactic SNRs have improved significantly over the past decade, allowing determination of radii (e.g., [34]). X-ray observations of SNRs have now been carried out for a significant fraction of Galactic SNRs. Previous work [23] improved the accuracy of spherically symmetric SNR evolution models by including results from a large grid of hydrodynamic simulations to develop the SNR modelling code SNRpy. Together, the new data and the modelling code enabled the application of SNR models for a large number of SNRs to derive their properties (e.g., [17]).

This work extends the calculations to include the XSPEC definitions which are commonly used by observers in deriving EM and kT_e from the X-ray spectrum. Although this makes little difference for FS gas, the difference is large for RS gas, and is required for correct interpretation of SNR properties derived from the RS gas. The process of including the XSPEC definitions in SNRpy is underway, and a new version is planned for release in mid-2022 on GitHub and on the website http://quarknova.ca.

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Notes

1 Calculated using the solar abundances from [32].

2 There are other cases where the integrals simplify, which we do not discuss in detail. e.g., if $\mu_{e,FS}(r)\mu_{H,FS}(r)$ = constant then EM_{FS} simplifies, and if $\mu_{e,FS}(r)\mu_{H,FS}(r)/\mu_{FS}(r)$ = constant then $kT_{EM,FS}$ simplifies. Similar special cases for other integrals are not discussed here.

3 We do not discuss other special cases which also give identical results, such as $kT_{e,EM,XS,FS} = kT_{e,EM,FS}$ for $(f_{T,FS}(r)\mu_{FS}(r))/(\mu_{e,FS}(r)\mu_{I,FS}(r)) =$ constant.

4 Otherwise, the more complicated full integral expressions must be used.

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