Understanding nebular spectra of Type Ia supernovae

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ABSTRACT

In this study, we present one-dimensional, non-local-thermodynamic-equilibrium, radiative transfer simulations (using CMFGEN) in which we introduce micro-clumping at nebular times into two Type Ia supernova ejecta models. We use one sub-Chandrasekhar (sub-M\(_{\text{Ch}}\)) ejecta with 1.02 M\(_{\odot}\) and one M\(_{\text{Ch}}\) ejecta model with 1.40 M\(_{\odot}\). We introduce clumping factors \(f = 0.33, 0.25, \) and 0.10 which are constant throughout the ejecta and compared to the unclumped \(f = 1.0\) case. We find that clumping is a natural mechanism to reduce the ionization of the ejecta, reducing emission from [Fe II], [Ar III], and [S III] by a factor of a few. For decreasing values of the clumping factor \(f\), the [Ca II] \(\lambda\lambda 7291,7324\) doublet became a dominant cooling line for our M\(_{\text{Ch}}\) model but still weak in our sub-M\(_{\text{Ch}}\) model. Strong [Ca II] \(\lambda\lambda 7291,7324\) indicates non-thermal heating in that region and may constrain explosion modelling. Due to the low abundance of stable nickel, our sub-M\(_{\text{Ch}}\) model never showed the [Ni II] 1.939 micron diagnostic feature for all clumping values.

Key words: keyword1 – keyword2 – keyword3

1 INTRODUCTION

The general consensus is that Type Ia supernovae (SNe Ia) are thermonuclear explosions of carbon-oxygen (C/O) white dwarfs (WDs) (Hoyle & Fowler 1960). Whether this explosion is the result of a system of one WD and a non-degenerate star (known as the single degenerate (SD) channel) or via a system of two WDs (known as the double degenerate (DD) channel) remains uncertain.

SNe Ia come from compact WDs and cool quickly via adiabatic expansion, and without an additional energy supply, they would be extremely difficult to detect. What powers the observed luminosity of SNe Ia is the decay of radioactive material produced during the explosion. The main radioactive isotope produced is \(^{56}\)Ni, whose decay chain is \(^{56}\)Ni \(\rightarrow ^{56}\)Co \(\rightarrow ^{56}\)Fe, releasing 1.72 and 3.75 MeV for each part of the decay chain. Therefore, the production of \(^{56}\)Ni is important in powering the luminosity of SNe Ia. However, the nickel yields (both stable and unstable) in SNe Ia are sensitive to both progenitor mass (\(\rho_p\)) and explosion scenario.

In 1D explosion modelling, higher central densities lead to enhanced electron capture and thus a larger neutron excess during the explosion. As a consequence, more stable nickel (\(^{58}\)Ni, \(^{60}\)Ni, and \(^{62}\)Ni) is produced (Nomoto 1984; Khokhlov 1991a,b). Sub-M\(_{\text{Ch}}\) WDs have lower central densities, and 1D modelling of SNe Ia from sub-M\(_{\text{Ch}}\) progenitors shows a lower abundance of \(^{58}\)Ni and \(^{60}\)Ni compared to M\(_{\text{Ch}}\) SNe Ia. However, 3D DDT modelling does not produce a \(^{56}\)Ni hole. Instead, the abundance of both \(^{56}\)Ni and \(^{58}\)Ni extend from the lowest velocities to about 10,000 km s\(^{-1}\) (Kasen et al. 2009; Seitenzahl et al. 2013). This result arises because ignition occurs in the centre of the WD. If ignition occurs on the surface, as in a double detonation, the burning front moves in and there is no mixing of stable Ni outwards (Woosley & Weaver 1994; Livne & Arnett 1995; Fink et al. 2007, 2010). Overall, the 3D simulations of WD explosions remain somewhat artificial, and the outcome depends strongly on number of ignition points and their distribution. Despite the time-scale for gravitational settling being ~ \(10^9 \sim 10^{10}\) yrs (Bildsten & Hall 2001), \(^{22}\)Ne settling in sub-M\(_{\text{Ch}}\) is proposed as a way to enhance the neutronization. Therefore, nebular nickel and IGE spectral features may constrain the physics of SNe Ia (Woosley 1997; Iwamoto et al. 1999; Stehle et al. 2005; Mazzali & Podsiadlowski 2006; Gerardy et al. 2007; Maeda et al. 2010a; Mazzali et al. 2011; Mazzali & Hachinger 2012; Mazzali et al. 2015).

Without knowing the progenitor system and explosion scenario, we fundamentally cannot accurately predict (despite understanding the flame physics) the amount of stable nickel produced, the overall abundances of IMEs, nor where in the ejecta these IMEs are produced relative to the \(^{56}\)Ni. However, studying nebular spectra will allow us to estimate these properties. At nebular times any nickel emission features are due to the remaining stable nickel, particularly from \(^{58}\)Ni and \(^{60}\)Ni. Since the width of any observed nebular feature is influenced by emission over the velocities at which the species exist, stable nickel features may help constrain the presence of the \(^{56}\)Ni hole (irrespective of the model).

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Nebular spectra are great tools to understand progenitors of SNe Ia. At this time, the ejecta is optically thin to continuum and most lines (with exceptions such as UV transitions), and much of the spectra comes from the inner part of the ejecta ($\lesssim 8000$ km s$^{-1}$), where the densities are highest and iron is the most abundant species. Because iron is most abundant in this region at nebular times, optical spectra are dominated by Fe II and Fe III lines and exhibit little to no flux from IME species such as S II and Ar III. The [Ca II] λ17291, 7324 may be blended with the [Fe II] λ17155, 7172, 7388 triplet, so its presence is difficult to determine.

Numerous previous studies have investigated SN Ia nebular spectra (Houck & Fransson 1992; Ruiz-Lapuente et al. 1992, 1993; Sm egreglia & Mazzali 1997; Mazzali et al. 1998; Gerardy 2002; Kozma et al. 2005; Maeda et al. 2010b; Blondin et al. 2012; Taubenberger et al. 2013b; Mazzali et al. 2015; Black et al. 2016; Botyánszki & Kasen 2017; Graham et al. 2017; Maguire et al. 2018; Black 2018; Diamond et al. 2018; Black et al. 2018). Authors often study emission lines by fitting Gaussian profiles to features that may or may not be blended. Maguire et al. (2018), for instance, fit Gaussian profiles to emission lines, and assumes the levels are in LTE with respect to the ground state. These authors also try and fit the complicated feature around 7300 Å without knowing the possibility of perturbation from IMEs.

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Previously theoretical modelling suggests clumping to be a byproduct of “nickel bubbles,” an expansion of the iron and nickel regions relative to the surrounding material due to radioactive decay energy deposition (Woosley 1988; Li et al. 1993; Basko 1994; Wang 2008). Rayleigh Taylor instabilities during DD burning (Golombek & Niemeyer 2005), or material interaction during detonation (Maier & Niemeyer 2006).

In this study, we strive for a model for the role of IMEs and the ionization structure by examining the influence of clumping. In this study, we use models SUB1 and CHAN from Wilk et al. (2018). In section 2 we discuss our technique for introducing clumping in our models. In section 3 we present the impact of clumping on nebular SN Ia spectra. We highlight the changes to the ionization structure in section 3.2. Shifts in ionization are reflected in some species, so in sections 3.3, 3.4, and 3.5 we discuss the effects on iron features, nickel features, and IMEs respectively. Finally, we summarize our work in section 4.

2 TECHNIQUE

2.1 Ejecta Models

This research uses two hydrodynamic models of Wilk et al. (2018), DDC10 (CHAN) and SCH5p5 (SUB1). DDC10 is a $M_{\odot}$ (1.40 $M_{\odot}$) model from Blondin et al. (2013). Model SCH5p5 is a sub-CC (1.04 $M_{\odot}$) from Blondin et al. (2017), but we have scaled the density by 0.98 (see Wilk et al. 2018) in order to have the same $^{56}$Ni. Both CHAN and SUB1 have the same $^{56}$Ni at 0.62 $M_{\odot}$. We use CMFGEN to solve the spherically symmetric, time-dependent, relativistic radiative transfer equation allowing for non-local thermodynamic equilibrium (non-LTE) processes. We take these two models at 216.5 days post-explosion from Wilk et al. (2018). Table 1 lists the initial masses for each model as well as the mass abundance of calcium, iron, cobalt, $^{58}$Ni plus $^{60}$Ni, and $^{56}$Ni. We see CHAN has more than twice the amount of stable nickel – $M_{\text{total}}$ – than SUB1 as well as almost a factor of two more calcium.

2.2 Numerical Treatment

Our original radiative-transfer calculations for our models did not include the effects of clumping. Therefore, to treat clumping in our models, we make some simple assumptions with CMFGEN. We assume there is no inter-clump media and the clumping is uniform in a homogeneous flow (i.e. $f/V = f_i$ for all species and velocities $V$). Assumptions underlying our clumping approach and discussions of the influence of clumping on core-collapse SNe II-P
are provided by Dessart et al. (2018). Our treatment of clumping in CMFGEN differs from that of a concentric shell-type structure, which is susceptible to radiative transfer effects across a shell and requires a large number of depth points to resolve the shells.

The clumping factor scales many variables, such as densities (scaled by $1/f$) and the emissivities and opacities (calculated using populations derived from clumps then scaled by $f$). This microclumping formalism leaves the mass column density unchanged. CMFGEN has incorporated this clumping method since Hillier & Miller (1999) first applied it to massive stars.

At a time step of 216.5 d post explosion ($\pm 200$ d post maximum) we resolved the relativistic radiative transfer equation for our models SUB1 and CHAN using a clumping factor ($f$) of 0.33, 0.25, and 0.1 (a value motivated by modelling of Wolf-Rayet stars (Hillier & Miller 1999)). Since the previous time-step was not computed using clumping in the models, we scaled the initial input populations by $1/f$ between successive ionizations. This simple scaling is adequate since time-dependent effects have a negligible influence on the spectrum.

3 RESULTS
Figs. 1 and 2 show the synthetic optical and near infrared (NIR) spectra of SUB1 and CHAN for the different values of a clumping factor ($f = 1.00, 0.33, 0.25$, and 0.10). In order to contrast the little amount of flux in the NIR, we show log $F_{\lambda}$ vs. $\lambda$ for wavelengths $1.0–2.4 \mu m$. We also show the component spectrum for $f = 0.10$ and $f = 0.33$ for models SUB1 and CHAN in Figs. 3, 4, 5, and 6.

3.1 Unclumped Models
Before we discuss clumping, it is necessary to understand and summarize the results of Wilk et al. (2018) that do not incorporate clumping. This Section focuses on two ejecta models, a direct detonation of a sub-M$_{\odot}$ WD and a DDT WD explosion model. Because our models come from two different explosion scenarios, the nucleosynthesis yields and stratification are model dependent. In 1D simulations of DDT explosions in M$_{\odot}$ WDs produce what is known as a $^{56}$Ni hole,” which is an underabundance of $^{56}$Ni in the innermost region. This arises due to neutron-rich nuclear statistical equilibrium (NSE) burning. Since our SUB1 model has lower central densities during explosion, it does not have a “$^{56}$Ni hole.” Therefore, SUB1 has a factor of about 2.26 less stable nickel.

Within the “$^{56}$Ni hole” of CHAN, the temperature and ionization is lower than in the region containing the original $^{56}$Ni.

Since stable nickel is centralized to the innermost part of the ejecta, it only becomes visible as the photosphere recedes inward and the ejecta becomes optically thin. Hence, the ejecta transitions into the nebular phase. Thus, nebular spectra allow us to probe this once shielded inner region. At 216 days post explosion (roughly +200 days post maximum), we do not see stable nickel in our SUB1 model, unlike in model CHAN. SUB1 has very little stable nickel in the inner region and also has Ni$_{2+}$ as its dominant ionization (see fig. 7 of Wilk et al. (2018)). At nebular times we expect to see forbidden [Ni II] lines, particularly [Ni II] $\lambda$7378, 7412 and [Ni II] $\lambda$1.939 $\mu m$, which are present in CHAN. Both models show strong emission from higher ionization states like Fe$^{2+}$, Co$^{2+}$, Ar$^{2+}$, and S$^{2+}$.

At nebular times, the energy deposited by radioactive decay is equal to the energy radiated by the gas by numerous cooling lines. In the models, radioactive decay heats both the IGEs as well as the IMEs. However, it is necessary to determine if these ejecta models will still show spectral signatures of IMEs when clumping is introduced.

3.2 Ionization Shifts
We show the average charge per species for sulfur, argon, calcium, iron, cobalt, and nickel for models with different amounts of clumping in Figs. 7 and 8. As expected, clumping shifts the ionization downward in both models for the IGEs from mostly doubly ionized to singly ionized (i.e. Fe$^{2+}$ → Fe$^{+}$). The strength of Fe III, Co III, Ni III, S III, and Ar III lines decreases considerably with increasing clumping, while Fe II and Co II lines increase. For both SUB1 and CHAN, the average charge of sulfur, argon, and cobalt differs by almost one electron between $f = 1.00$ and $f = 0.10$ in the inner ejecta regions.

3.3 Impact on Iron Lines
Figs. 1 and 2, show that the Fe I, Fe II, and Fe III optical features changed significantly. The [Fe III] $\lambda$4658, 4702 feature dropped in flux by more than a factor of two in both ejecta models from $f = 1.00$ to $f = 0.10$, while we saw the emergence of Fe I features between 4100–4500 Å and between 5400–5600 Å ($\lambda \lambda$4375, $\lambda$4385, $\lambda$4395, and Fe II) for clumping. Figs. 1 and 2 show the Fe I emission as a shoulder to the neighboring [Fe III] and [Fe II] emission for $f = 0.33$ and 0.25, while we see a noticeable peak for $f = 0.10$.

While Fe II features were generally enhanced, the expected Fe II feature around 4359 Å (believed to be the $^{56}$Fe$^{2+}$ transition and similarly the $^{56}$Fe$^{-D_2}$ transition at $4287$ Å) is weak or absent in our models compared with observations. An examination of the individual Fe I, Fe II, and Fe III spectra showed that the optical depth effects are important. It appears that the emergence of partially thick Fe 1 lines, Ti II lines like 4395 Å, and permitted Fe II lines reduce the strength of the claimed [Fe II] $\lambda44287$, 4359 doubelt believed to be seen in nebular spectra.

In Figs. 9, 10, and 11 we show the optical depth to the [Fe II] $\lambda$4359 resonance zone (at velocity V) arising from interactions with other lines along the line of sight. There are tens of interacting lines to the outer ejecta and ~25 000 interacting lines to the inner ejecta. Figs. 9 and 10 show this optical depth (and the continuum optical depth) along a core ray through the ejecta. The line transitions with the largest optical depth contributions are Fe I ($\lambda$4384, Fe I $\lambda$4375, Ti I $\lambda$4395, Fe II $\lambda$4385, and Fe I) $\lambda$4404. Differences between models and levels of clumping reflect the differences in the ionization of iron since the largest contributions to the optical depth primarily come from iron lines. Fig. 11 shows this optical depth along various rays parallel to the z-axis towards the observer ($v_y$ and $v_z$). In both models, [Fe I] $\lambda$4359 reaches an optical depth of unity at roughly 10 000 km s$^{-1}$ for a clumping factor of 0.10. In model CHAN, the Sobolev line optical depth reaches unity around 5 000 km s$^{-1}$ for $f = 0.33$, while for model SUB1 it is true around 2500 km s$^{-1}$. Figs. 1 and 2 highlight how little flux is seen below 4500 Å.

Studies of SN Ia nebular spectra often investigate the [Fe II] feature around 12 600 Å (Maguire et al. 2018; Diamond et al. 2018) since it is the least blended feature in nebular SN Ia spectra (free from other lines and ionization states of Fe). Our models confirm it is “blend-free” line complex is therefore the best feature to constrain the Fe II emitting region. We show in Fig. 12 that this
[Fe II] feature can be reproduced by calculating an emission spectrum. To produce this emission spectrum, we use the temperature and ionization structure from CMFGEN and re-solve the level populations considering only collisional processes and radiative decays. The relativistic radiative transfer equation is then solved assuming zero opacity. We show this line complex can be inferred from tomography, as it is only sensitive to the temperature and ionization. However, this method will break down for departures from spherical symmetry.

Various observations of nebular SN Ia spectra show a slight shouldershading on the 4600 Å iron complex due to a potential Fe I feature at 5500 Å – z 5\text{D} \rightarrow a 5\text{F} (\text{Fe}) optical transitions – (Childress et al. 2015; Graham et al. 2017). Such Fe I features could constrain the level of ionization within SN ejecta and assist future modelling. Since Fe I features cause optical depth effects with [Fe II] \lambda 4287, 4359, it is important to determine the Fe II ionization. Despite all the observations showing [Fe II] \lambda 4287, 4359, this feature has yet to be accurately modelled by other researchers (Spyromilio 2016, private communication; Sim 2016, private communication). Shifts in the ionization of (Fe\text{II} \rightarrow Fe^+) are expected as the ejecta continues expands and cools as less energy is deposited from radioactive decays (Fransson & Jerkstrand 2015). Fransson & Jerkstrand (2015) showed that at very late times (1000 days), the 4600 Å iron complex, despite its similar appearance to early epochs, is dominated by emission from Fe I and Fe II.

3.4 [Ni II] 1.939 microns

In SUB1 models, the ionization fraction for nickel (Ni\text{II} / Ni\text{II}) drops in the inner region (\lesssim 5000 km s^{-1}) by roughly three orders of magnitude when changing f = 1.0 to f = 0.10. However, the [Ni II] 1.939 Å line is still absent in SUB1. Where the line formation occurs, below \sim 6500 km s^{-1}, the electron density is higher than 10^{3} cm^{-3} in the inner part of the ejecta, so its line emission scales linearly with density as we increase the amount of clumping. These densities are above the critical density for the upper level of this transition, so collisional de-excitation are important.

With f = 0.10 for SUB1, the weak [Ni II] 1.939 micron line is also a factor of a few weaker than \text{[Ca II]} 1.9035 microns. SUB1 has more than a factor of 2 less stable nickel compared to CHAN (Table 1) in which we do still see the [Ni II] 1.939 micron line. With all of these factors such as ionization and abundance accounted for, it is not surprising that spectra of SUB1 still do not show this line.

3.5 IMEs

Due to the overlap in production/mixing of 56Ni and IMEs in our models, the strengths of IMEs are sensitive to the non-thermal heating and ionization structure within the ejecta. Within our models, a consequence of clumping is the enhancement of the [Ca II] \lambda 7291, 7324 doublet. The [Ca II] doublet is blended with the [Fe II] \lambda 7155, 7172, 7388 triplet and [Ar III] \lambda 7136, and it contributes a large portion of the flux to the blended feature (see Figs. 3-6). The [Ca II] emission flux is model dependent. Not only is the mass of calcium \sim 1.75 times larger in CHAN than SUB1 but also the distribution of calcium varies significantly between SUB1 and CHAN. In SUB1, the inner region containing 80 percent of the energy deposited only contains 25 percent of the calcium mass. In CHAN, however, the inner region containing 80 percent of the energy deposited contains 50 percent of the calcium mass. These models help constrain the amount of stratification between the original 56Ni and IMEs required to produce SNe Ia nebular spectra.

Once the ionization is lowered, Ca\text{II} becomes the dominant cooling for the zone rich in IMEs, since S\text{II} and Ar\text{II}, unlike their twice-ionized siblings, do not have strong cooling lines due to their low critical densities. We see the strength in the twice-ionized sulfur and argon lines ([S III] \lambda 4906, 9530 and [Ar III] \lambda 7175, 7751) decreases as we lower the clumping factor. However, it is unclear if such strong [Ca II] \lambda 7291, 7324 emission is seen in spectra of classic SNe Ia blended into the feature around 7200 Å, which is thought to be mostly [Fe II] and [Ni II], in nebular spectra – Taubenberger et al. (2015a); Bikmaev et al. (2015); Graham et al. (2017); Maguire et al. (2018). For low luminosity 91bg-like SNe Ia (such as SN1999by), modelling suggests Ca emission is the dominant contributor of the 7200 Å feature at \sim 180 days (Blondin et al. 2018).

If the 7200 Å feature is highly blended with [Ca II], then for a given electron density and temperature, we can predict emissivity per ion ratio of the [Ca II] doublet to the [Fe II] lines using some simple physical assumptions. Assuming only collisional processes and radiative decays, we can solve for the atomic level populations for a range of temperatures and electron densities. Fig. 14 shows the emissivity ratio of the [Ca II] \lambda 7291 transition to the [Fe II] \lambda 7155 transition for a range of temperatures and electron densities with our simple assumptions. As shown in Fig. 14, for equal N(Fe\text{II})/N(Ca\text{II}) = 1, the emissivity ratio between [Ca II] \lambda 7291 and [Fe II] \lambda 7155 for temperatures between 2000-7000 K and electron densities between 10^{5}-10^{6} cm^{-3} is between a factor of 10-100. However, in our models, our N(Fe\text{II})/N(Ca\text{II}) is \sim 5-30 between 5000-10000 km s^{-1}. Therefore, we expect to see [Ca II] \lambda 7172, 7324 emission blended as long as the N(Fe\text{II})/N(Ca\text{II}) is \lesssim 100. Although this only relates to the stronger component of the [Ca II] doublet, the [Ca II] \lambda 7324 line comprises roughly 40 percent of the overall contribution from [Ca II] (see Table 2). The other [Fe II] blended components will contribute much less flux as the Einstein A values are a factor of 2-3 less than the [Fe II] \lambda 7155 transition.

Despite the level excitation energy of Ca\text{II} \lambda 2\text{D} \rightarrow g\text{2G} and Fe\text{II} \lambda 2\text{D} \rightarrow g\text{2G} being similar (\sim 16 percent difference), the average level populations in LTE can be several orders of magnitude different for the same total ion population. The average LTE level population compared to the total is simply

\[
\frac{N(\text{Fe}\text{II}[\lambda 2\text{G}])}{N(\text{Fe}\text{II})} = \frac{1}{Z} \int_{0}^{\infty} \text{g} \cdot \text{E}[\lambda 2\text{G}] / kT dE,
\]

where Z is the partition function. For temperatures of 2000, 5000, and 10000 K, the partition function (using the first 18 levels) is approximately 28, 43, and 58 respectively assuming the states are in LTE with respect to the ground state. Since Fe\text{II} has many easily excited lower levels, then even for the same ion abundance between Ca\text{II} and Fe\text{II}, the emission from Ca II will dominate the blended feature at 7200 Å.

The strong emission of the [Ca II] \lambda 7172, 7324 doublet is not only a result of the ionization, temperature, and electron density but also coupled to the radiation field. The Ca II H & K lines have large oscillator strengths and can pump electrons into the upper \text{2P}\text{I} levels. They then decay to the \text{2S} ground state giving us [Ca II] \lambda 7172, 7324 emission. We have taken our ionization, temperature, and electron density structure from CMFGEN and re-solved for the level populations of Ca\text{II} assuming only collisional and radiative decay processes. For levels that are coupled to UV transitions, this assumption is only accurate within 50%. We then solved the relativistic radiative transfer equa-
tion for line emission of Ca II with zero opacity. Our results (see Fig. 12) show the spectra of Ca II is sensitive to the radiation field. Flux is absorbed in the Ca II H&K lines which can then be emitted in the Ca II NIR triplet as well as the [Ca II] λλ 4227, 4371 doublet. Despite the critical densities for Ca II 3D/2 and 1D being on the order of ~ 10^9 - 10^10 cm^-3, the atomic levels above the Ca II 3D/2 and 1D have sufficiently high critical densities which inhibits collisional de-excitation locking these levels to their LTE value.

Such strong [Ca II] emission could indicate a problem with our atomic data for Fe I/Fe II or likely be an indication of more stratified material in our 1D models. Element stratification within the ejecta also influences the strength of the lines belonging to IMEs. In particular, the presence of some 56Co in the IME zone means that positrons are available as a heating source after the ejecta has become optically thin to γ-rays. However, even at late times, this contributes only a fraction of non-thermal heating in the inner region. γ-rays still scatter out into the ejecta, heating some of the outer layers.

If the problem lies not with our atomic data, then stratification is the cause of strong IME emission. This puts a constraint on the nucleosynthetic distribution of calcium produced in SNe Ia. This either prohibits an overlap between the calcium and the radioactive nucleosynthetic distribution of calcium produced in SNe Ia. This is the cause of strong IME emission. This puts a constraint on the average ionization of IMEs in the inner region. If the problem lies not with our atomic data, then stratification is the cause of strong IME emission. This puts a constraint on the nucleosynthetic distribution of calcium produced in SNe Ia. This either prohibits an overlap between the calcium and the radioactive nucleosynthetic distribution of calcium produced in SNe Ia. This is the cause of strong IME emission. This puts a constraint on the average ionization of IMEs in the inner region.

4 CONCLUSION

We have performed 1D radiative transfer calculations using CMFGEN for two ejecta models (one sub-M Chandeleur detonation and one M Chandeleur DDT – see Wilk et al. (2018) for more details) utilizing micro-clumping at 216.5 days post explosion. Our goal was to understand the influence of micro-clumping on nebular spectra and to test when clumped models would provide a better fit to the observed level of ionization in Ia spectra. Clumping is expected to occur naturally in SN ejecta and naturally reduces the ionization by enhancing recombination. We considered three different clumping factors, 0.33, 0.25, and 0.10, which we assumed were constant throughout the ejecta. Our models are in a regime where potentially small changes can shift the ionization. This also means that our models are sensitive to atomic physics.

Clumping lowers the average ionization of all species. The average ionization of IMEs is reduced by about one electron below 10,000 km s^-1 and roughly one half of an electron for IGEs (except cobalt which is reduced by roughly an electron). Despite clumping lowering the ionization in SUB1, the nickel ionization remained high in the inner region due to a lack of a ~56Ni hole.” With an already reduced stable nickel mass compared to CHAN, SUB1 failed to show strong emission from Ni II in the optical and in the NIR with the [Ni II] λ 1.939 μm line.

As iron is the most abundant species in the inner ejecta at 216 days, clumping had the most visible effect on the flux of [Fe III] features such as [Fe III] λλ 4465, 4702. As the iron ionization is lowered, the flux in Fe III features increases, and permitted Fe I lines near 5500 Å emerged. These Fe I lines cause a shoulder to form on the [Fe II] and [Fe III] optical blend between 4200-5400 Å. Our attempts to model the [Fe II] λλ 4428, 4359 feature were unsuccessful. While clumping generally enhanced the strength of [Fe II] features, absorption by other transitions limit its strength. Despite the difficulty in reproducing [Fe II] λλ 4428, 4359, we show that the [Fe II] complex around 12500 Å is completely reproduced under simple physics assumptions of collisional and radiative decays from a given ionization and temperature structure. In the IR, particularly from 10,000-11,800 Å, changes in the flux of Fe I lines of several orders of magnitude for a factor of a few change in density. For the same 56Ni mass, M Chandeleur explosions produce more IMEs compared to sub-M Chandeleur explosions. We have seen that only large clumping can sufficiently suppress emission from IMEs such as Ar III and S III. However, as we increase clumping, both models show an increase in the [Ca II] λλ 4227, 4371, which dominates over the [Fe II] λ 17155 feature. Since the presence/absence of [Ca II] in this 7200 Å blend is still highly uncertain, we suggest that SN Ia ejecta require less mixing between the original 56Ni and the calcium distribution. Another possibility is that the Ni and Ca are not microscopically mixed. In that case non-thermal energy deposited in the Fe region would be radiated by Fe, while the energy deposited in the IME region would be radiated primarily by IMEs. In this case the strength of the [Ca II] lines relative to [Fe II] would be set by the amount of heating in each region.

Despite arguments that mixing is required to reproduce early-time LCs, mixing between layers of IMEs and 56Ni is inconsistent with what is observed at nebular times, since the emission reflects where most of the energy is deposited. The strength of time-dependent IME features in nebular spectra is a crucial diagnostic for understanding both progenitors and explosion properties of SNe Ia.

Better atomic data can also assist determining the sensitivity it has on the Fe I/Fe II/Fe III features in producing nebular spectra. Because the focus of this work is on nebular phase modelling, further work is necessary to test the time-dependent effects of various levels of clumping. It would be helpful to perform full time-series calculations. Clumping should be fully explored to truly understand the nature of the progenitors of SNe Ia.
### Table 1.

Model mass information in $M_⊙$ at 0.75 days post explosion. The parentheses (#) correspond to $\times 10^9$.

| Model | $M_\text{SUB1}$ | $M_\text{CHAN}$ | $M_\text{Ca}$ | $M_\text{Fe}$ | $M_\text{Co}$ | $M_\text{56Ni} + M_\text{56Ni}$ | $M_\text{56Ni}$ |
|-------|----------------|----------------|----------------|----------------|---------------|-----------------------------|---------------|
| SUB1  | 1.04           | 1.046(-1)      | 2.273(-2)      | 2.361(-2)      | 2.226(-2)     | 1.113(-2)                  | 5.684(-1)     |
| CHAN  | 1.40           | 1.661(-1)      | 3.693(-2)      | 4.120(-2)      | 1.020(-1)     | 5.713(-2)                  | 5.708(-1)     |

### Table 2.

The parentheses (#) correspond to $\times 10^8$. $T_4$ is just $T/(10^4 \text{K})$.

| Term | Upper level $u$ | Lower level $l$ | $A_{ul}$ (s$^{-1}$) | Wavelength (Å) | $N_{\text{crit}}(T_4 = 0.1)$ (cm$^{-3}$) | $N_{\text{crit}}(T_4 = 0.5)$ (cm$^{-3}$) | $N_{\text{crit}}(T_4 = 1.0)$ (cm$^{-3}$) |
|------|----------------|----------------|---------------------|----------------|-------------------------------------------|-------------------------------------------|-------------------------------------------|
| Ca$^+$ | Term | $g$ | $E_u$ (eV) | Term | $g'$ | $E_l$ (eV) | |
| $^{2}D_{5/2}$ | 6 | 1.699932 | $^{2}S_{1/2}$ | 2 | 0.000 | 8.025(-1) | 7291.469 | 7.722(5) | 1.717(6) | 2.125(6) |
| $^{2}D_{3/2}$ | 4 | 1.692408 | $^{2}S_{1/2}$ | 2 | 0.000 | 7.954(-1) | 7323.888 | 6.070(5) | 1.290(6) | 1.645(6) |
| Fe$^+$ | Term | $g$ | $E_u$ (eV) | Term | $g'$ | $E_l$ (eV) | |
| $a^{2}G_{9/2}$ | 10 | 1.96448603 | $a^{4}F_{9/2}$ | 10 | 0.23217278 | 1.4950(-1) | 7155.157 | 5.165(6) | 9.130(6) | 9.618(6) |
| $a^{2}G_{7/2}$ | 8 | 2.02954814 | $a^{4}F_{7/2}$ | 10 | 0.30129857 | 5.6950(-2) | 7172.004 | 2.415(6) | 4.010(6) | 4.207(6) |
| $a^{2}G_{7/2}$ | 8 | 2.02954814 | $a^{4}F_{5/2}$ | 6 | 0.381586476 | 4.3450(-2) | 7388.178 | 2.415(6) | 4.010(6) | 4.207(6) |
| $a^{2}G_{9/2}$ | 10 | 1.96448603 | $a^{4}F_{7/2}$ | 10 | 0.30129857 | 4.8450(-2) | 7452.538 | 5.165(6) | 9.130(6) | 9.618(6) |
Figure 1. Spectra of SUB1 at 216.5 days post-explosion compared to the spectra computed using different clumping factor values (0.33, 0.25, and 0.1). The spectra have all been scaled by the same value. To contrast the little flux in the IR, we show the logarithm of the flux. In the IR, particularly from 10 000-11 800 Å, changes are several orders of magnitude for a factor of a few in density.
Figure 2. Spectra of CHAN at 216.5 days post-explosion compared to the spectra computed using different clumping factor values (0.33, 0.25, and 0.1). The spectra have all been scaled by the same value (and also to Fig. 1). To contrast the little flux in the NIR, we show the logarithm of the flux. Differences between the spectra can be large (greater than a factor of 10) for Fe I and Fe II features for just a factor of 3 or more in density.
Figure 3. Observer’s frame spectrum (thick black line) of SUB1 along with the component spectra of Fe I, Fe II, Fe III, Co II, Co III, Ni II, Ni III, Ca II, S III, and Ar III at 216.5 days post-explosion for a clumping factor of $f = 0.10$. If the optical depth effects are unimportant, the component spectrum will sum to the total to produce the full spectrum (thick black line). Conversely, we see that the features between 4000-5500 Å cannot be understood without allowing for optical depth effects.
Figure 4. Observer’s frame spectrum (thick black line) of SUB1 along with the component spectra of Fe i, Fe ii, Fe iii, Co ii, Co iii, Ni ii, Ni iii, Ca ii, S iii, and Ar iii at 216.5 days post-explosion for a clumping factor of \( f = 0.33 \). If the optical depth effects are unimportant, the component spectrum will sum to the total to produce the full spectrum (thick black line). Conversely, we see that the features between 4000-5500 Å cannot be understood without allowing for optical depth effects.
Figure 5. Observer’s frame spectrum (thick black line) of CHAN along with the component spectra of Fe I, Fe II, Co II, Ni II, Ni III, Ca II, S III, and Ar III at 216.5 days post-explosion for a clumping factor of \( f = 0.10 \). If the optical depth effects are unimportant, the component spectrum will sum to the total to produce the full spectrum (thick black line). Conversely, we see that the features between 4000-5500 Å cannot be understood without allowing for optical depth effects.
Figure 6. Observer’s frame spectrum (thick black line) of CHAN along with the component spectra of Fe i, Fe ii, Fe iii, Co ii, Co iii, Ni ii, Ni iii, Ca ii, S iii, and Ar iii at 216.5 days post-explosion for a clumping factor of $f = 0.33$. If the optical depth effects are unimportant, the component spectrum will sum to the total to produce the full spectrum (thick black line). Conversely, we see that the features between 4000-5500 Å cannot be understood without allowing for optical depth effects.
**Figure 7.** Model SUB1 average charge on species for sulfur, argon, calcium, iron, cobalt, and nickel for clumping factors of 1.00, 0.33, 0.25, and 0.10 at roughly +200 d after maximum. The ionization is largely sensitive to the clumping factor and the non-thermal energy deposition in the inner ejecta. Sulfur and argon show changes of roughly one electron, while iron shifts from mostly Fe$^{2+}$ to nearly equal parts Fe$^{2+}$ and Fe$^+$. The majority of the stable nickel is located in the inner ejecta, and in this region the ionization is driven by the radioactive decay deposition. These changes in the inner region relate to large changes on the spectra.
Figure 8. Same as Fig. 7 but for model CHAN. The changes in the ionization are smallest (except for calcium) in the region of the \(^{56}\text{Ni} \text{hole}\) between different amounts of clumping. The slope of the average ionization of iron and other species in the inner region highlights that small changes can shift the ionization.
Figure 9. The optical depth to $[^{\text{Fe}}\text{II}]$ $4359\AA$ resonance zone at velocity $V$ for various clumping factors for SUB1. We consider this along the first core impact parameter ($p_1 = 0$). The dashed lines correspond to the sum total of all lines that interact with the $[^{\text{Fe}}\text{II}]$ $4359\AA$ line emitted at a particular resonance zone. The dotted lines correspond to the continuum contribution, and the solid lines represent the total $[^{\text{Fe}}\text{II}]$ $4359\AA$ optical depth to the resonance zone.

Figure 10. Same as Fig. 9 but now for model CHAN.
Figure 11. The 2D optical depth of the [Fe II] $\lambda$4359 (just as in Figs. 9 and 10) along rays parallel to the z-axis for various impact parameters (y-direction). We only consider interacting lines whose Sobolev optical depth at their resonance zone is greater than $10^{-5}$. We interpolate the results from our 1D grid onto a rectangular grid. The white space is where the optical depth is zero.
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Figure 12. Observer’s frame emission spectra of Fe II, Fe III, Ni II, Co II, Co III, and Ca II. We show the full observer’s frame spectrum in black. The emission spectra are calculated by taking the temperature and ionization structure output from CMFGEN and re-solving the level populations assuming only collisional processes and radiative decays. We assume Gaussian emission profiles of 100 km s$^{-1}$ in the CMF.

Figure 13. Left plot is the mass fractions for calcium and iron in both models. The solid line corresponds to model CHAN, and the dashed line corresponds to SUB1. The right plot is the cumulative distribution function for the energy deposition (solid lines) and the calcium mass (dashed lines) at 217 days after explosion (roughly +200 days).
Figure 14. Line emission ratio of the [Ca II] $\lambda$7291 to [Fe II] $\lambda$7155 assuming $N(\text{Fe}^+)/N(\text{Ca}^+) = 1$. The emission ratio is calculated by solving the rate equations with only collisional and radiative decay terms for a fixed ionization of $N(\text{Fe}^+)/N(\text{Ca}^+) = 1$. The emission ratio favors strong calcium. When this ionization ratio is $\gtrsim 50$ the iron would begin to dominate the 7200 Å complex.