

Revisiting the formation of molecules and dust in core collapse supernovae

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ABSTRACT

Context. Core-collapse Supernovae (CCSNe) classed as Type II contribute to the chemical enrichment of galaxies through explosion. Their role as dust producers in the high-redshift Universe may be of paramount importance. However, the type and amount of dust they synthesise following the outburst are still a matter of debate and their formation processes also remain unclear.

Aims. We aim to identify and understand the chemical processes at play in the dust formation scenario. We also derive mass yields for molecules and dust clusters at late post-explosion time.

Methods. We revisited existing models by improving on the physics and chemistry of the supernova ejecta. We identified and evaluated new chemical species and pathways underpinning the formation of dust clusters. We applied a unique exhaustive chemical network to the entire ejecta of a SN with a 15 M_⊙ progenitor. We tested this new chemistry for various gas conditions in the ejecta, and derived mass yields for molecules and dust clusters.

Results. We obtained the molecular component of the ejecta up to 11 years after explosion. The most abundant species are, in order of decreasing masses, O₂, CO, SiS, SiO, CO₂, SO₂, CaS, N₂, and CS. Atomic oxygen is quickly depleted after 300 days post-explosion in a large part of the oxygen core owing to the efficient synthesis of O₂. Caution should then be exercised in the use of atomic oxygen masses as a supernova diagnostic. We identified molecules that are tracers of high-density clumps. As for dust clusters, we find the composition is dominated by silicates and silica, along with carbon dust, but with modest amounts of alumina. Pure metal clusters and metal sulphide and oxide clusters have negligible masses. High-density gas favours the formation of carbon clusters in the outer ejecta region whereas low temperatures hamper the formation of silicates in the oxygen core. These results are in good agreement with existing astronomical data and recent observations with the James Webb Space Telescope (JWST). They highlight the importance of chemistry in the derivation of dust budgets from supernovae.

Key words. astrochemistry – molecular processes – supernovae: general

1. Introduction

Supernovae (SNe) hold a special place among the dust contributors to galaxies. Indeed, the explosion of massive stars with initial masses on the zero age main sequence (ZAMS) of between 8 M_⊙ and 30 M_⊙ leads to dust formation in the ejected gas (i.e. ejecta). However, the exact dust amount that is formed following the outburst is still a matter of debate. Determining the SN dust yields is of paramount importance for assessing the dust budgets of local and high-redshift galaxies and the competition as dust providers between SNe and evolved, low-mass stars on the asymptotic giant branch (AGB). According to several studies, SNe may represent the main dust factories in primeval galaxies at high redshift (Dwek & Cherchneff 2011; Schneider & Maiolino 2024), but the contribution of AGB stars may be more important than initially estimated (Boyer et al. 2025). Despite the huge amount of energy released by the explosion ($\sim 1 B = 1 \times 10^{51}$ Erg) and the harsh physical conditions experienced by the ejecta, for many SNe, the presence of molecules and dust can be inferred a few hundred days after the explosion.

The explosion of the blue supergiant Sanduleak–69 202 in the Large Magellanic Cloud more than 35 years ago, leading

to SN1987A, provided the first evidence of molecule and dust synthesis in SN ejecta. The fundamental and overtone transitions of carbon monoxide, CO, and the fundamental transition of silicon monoxide, SiO, were detected as early as 120 days post-explosion (i.e. day 120) (Catchpole et al. 1988; Spyromilio et al. 1988; Meikle et al. 1989; Roche et al. 1991), while an asymmetry of optical emission lines combined with a decrease in luminosity were interpreted as evidence of dust production at day 530 (Lucy et al. 1989; Danziger et al. 1991). Since then, emission lines of CO, SiO, SO, SO₂, and HCO⁺ (and, possibly, SiS) were detected in the young remnant of SN 1987A with the Atacama Large Millimetre/sub-millimetre Array, ALMA (Kamenetzky et al. 2013; Matsuura et al. 2017; Cigan et al. 2019). Other Type II SNe were investigated with the detection of CO and/or SiO molecules, along with evidence of dust formation a few hundred days after the outburst (e.g. Kotak et al. 2005, 2006, 2009; Rho et al. 2018; Park et al. 2025; Medler et al. 2025).

A direct proof of the existence of dust grains produced in SNe has been delivered by studies of primitive Solar System materials (e.g. meteorites and interplanetary dust). The extracted pre-solar grains show anomalies in their isotopic composition characteristics of the nucleosynthesis of their parent stars. Pre-solar grains with SN origin include mainly silicates, with most grains having compositions consistent with olivine

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(e.g. forsterite Mg_2SiO_4) or pyroxene (e.g. enstatite MgSiO_3), or intermediate between these two, along with graphite and (to a lesser extent) silicon carbide, as well as metal oxides such as alumina (Al_2O_3) and spinel (MgAl_2O_4). Rare pre-solar grains with SN origin such as silicon nitride (Si_3N_4) and silica (SiO_2) have also been identified (Nittler et al. 1995; Haenecour et al. 2013).

The first exhaustive physico-chemical models of molecule and dust formation in SN ejecta showed that specific molecules such as O_2 , CO , SiO , and SO form in large quantities about 100 days after explosion in local and high-redshift SNe (Cherchneff & Lilly 2008; Cherchneff & Dwek 2009, 2010; Sarangi & Cherchneff 2013). In the case of SN1987A, the predicted large CO mass of $\sim 0.1 M_\odot$ was confirmed by ALMA observations (Kamenetzky et al. 2013). The molecular component of the ejecta represents between 10–40% of the ejected matter, depending mainly on the progenitor mass and ^{56}Ni content (Cherchneff & Dwek 2009; Sarangi & Cherchneff 2013). Along with molecules, these models predict the synthesis of large quantities of dust equivalent to $\sim 8\%$ and $\sim 2\%$ of the ejecta mass for high- z pair instability and local Type II SNe, respectively (Cherchneff & Dwek 2010; Sarangi & Cherchneff 2015), with dust compositions including silicates, alumina, silica, and carbon. Further studies of SN1987A that have been based on a comparable approach (Sluder et al. 2018) and using a similar chemical network (Sarangi 2022) corroborate these findings for local SNe. However, there are several drawbacks and simplifications in the existing chemical models. For example, different chemical schemes are applied to the various ejecta regions while most of the nucleation pathways and reaction rates for dust clusters are greatly optimised.

The present study is the first in a series of new investigations on molecule and dust formation in local and high- z SNe. Here we revisit the chemistry of a non-interacting Type II SN of progenitor mass equals to $15 M_\odot$. We aim to shed light on the processes at the origin of the formation and evolution of molecules and the nucleation of dust in the nebular phase. In doing so, we consider a large number of new chemical species and processes not included in previous studies and we define one unique chemical scheme that we apply to the entire ejecta. We re-investigate dust nucleation routes in light of recent theoretical and experimental studies for several dust types, thereby greatly improving on previous chemical descriptions of dust synthesis. This new model confirms the presence of already detected key molecules and predicts new species widely present in the ejecta. We assess dust masses and point to specific ejecta conditions necessary to foster the production of silicate and carbon dust. In the era of the James Webb Space Telescope (JWST), we believe this new model provides useful information to be used in the interpretation of current and future astronomical data. The improved physical and chemical models are described in Sects. 2 and 3, while the results are presented and discussed in Sect. 4, along with a comparison to observations and exiting studies in Sects. 5 and 6. Finally, our conclusions are outlined in Sect. 7.

2. The physical model

We chose a $15 M_\odot$ stellar progenitor as a template in this study. This mass is in line with the progenitor masses proposed for several Type IIP SNe recently observed and monitored by JWST, such as SN 2017eaw (Kilpatrick & Foley 2018; Szalai et al. 2019) and SN 2023ixf (Van Dyk et al. 2024). Larger and smaller progenitor masses will be investigated in a future study.

We then assumed the ejecta remain spherical and stratified after explosion although SN ejecta are expected to be

Table 1. Parameters for the $15 M_\odot$ ejecta (Rauscher et al. 2002).

t_0	E_{ex}	M_{He}	v_{He}	v_c	$\rho_{\text{gas}}(t_0)$
100 (days)	1.2 (B)	4.23 (M_\odot)	2274 ^a (km s^{-1})	3522 ^a (km s^{-1})	1.35×10^{-13} (g cm^{-3})
Isotope i	$1/\lambda_i$ (days)	M_i^b (M_\odot)	E_i^{c} (MeV)	κ_i^d ($\text{cm}^{-2}\text{g}^{-1}$)	$\tau_{i,0}$ –
^{56}Co	111.43	0.1261	3.606	0.033	17.17
^{57}Co	392.04	4.211×10^{-3}	0.1216	0.0792	41.21
^{44}Ti	31121.10	3.421×10^{-5}	2.275	0.04	20.81

Notes. ^(a) See Equations 10 and 13 below; ^(b) Rauscher et al. (2002); ^(c) Seitzzahl et al. (2014); ^(d) Woosley et al. (1989).

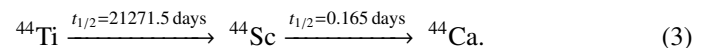
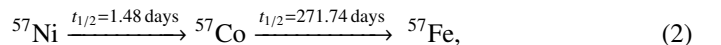
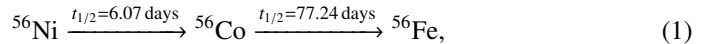
clumpy and asymmetric, as shown by 3D explosion models (Kifonidis et al. 2006; Wongwathanarat et al. 2015). Although macroscopic mixing of hydrogen down to the ejecta core is observed (Utrobin et al. 2019), we assumed hydrogen was not microscopic mixed within our stratified core. Therefore, the derived molecule and dust compositions of the various regions within our stratified core apply to ejecta clumps and hint at local yields, while absolute yields depend on clumping. Since there is no information on the ejecta gas parameters for our SN template, we built our model by using information on other SN ejecta (e.g. SN1987A). We then used our composite model to test the new proposed chemistry.

2.1. Initial conditions

The chemical and physical parameters characterising the explosion of our $15 M_\odot$ template were taken from Rauscher et al. (2002) and correspond to the model s15a27c¹, for which the kinetic energy of the explosion is 1.2 B.

Radioactive elements, such as ^{56}Ni , ^{56}Co , and ^{44}Ti , create a flux of γ -ray photons that pervades the ejecta. The degrading of γ -rays to X-rays and ultraviolet (UV) photons occurs by Compton scattering and creates a population of fast Compton electrons in the ejecta. These fast electrons directly destroy molecular species and ionise the gas to produce noble gas ions such as Ar^+ , Ne^+ , and He^+ , which are key species to the ejecta chemistry.

To estimate the ionisation rates of Compton electrons in Sect. 3, we first need to assess the radioactive energy deposition rate in the ejecta. The SN light curve is powered by the radioactivity of several decay chains, among which the most important for our study are listed below with the corresponding half-lives $t_{1/2}$ ²



For an isotope, i , the energy deposition rate through radioactive decay and emission of γ -rays at a time, t , is given by

$$L_i(t) = \lambda_i N_i(0) e^{-\lambda_i t} (1 - e^{-\tau_{i,0}(t/t_0)^{-2}}) E_i^\gamma \quad (4)$$

where $\lambda_i = \ln(2) / t_{1/2,i}$ is the decay constant, $N_i(0)$ is the total number of isotope, i , at a time, $t = 0$, $\tau_{i,0}$ is the optical depth

¹ Data can be retrieved at <https://nucastro.org>

² Information extracted from the NuDat database, National Nuclear Data Center, <https://www.nndc.bnl.gov/nudat>

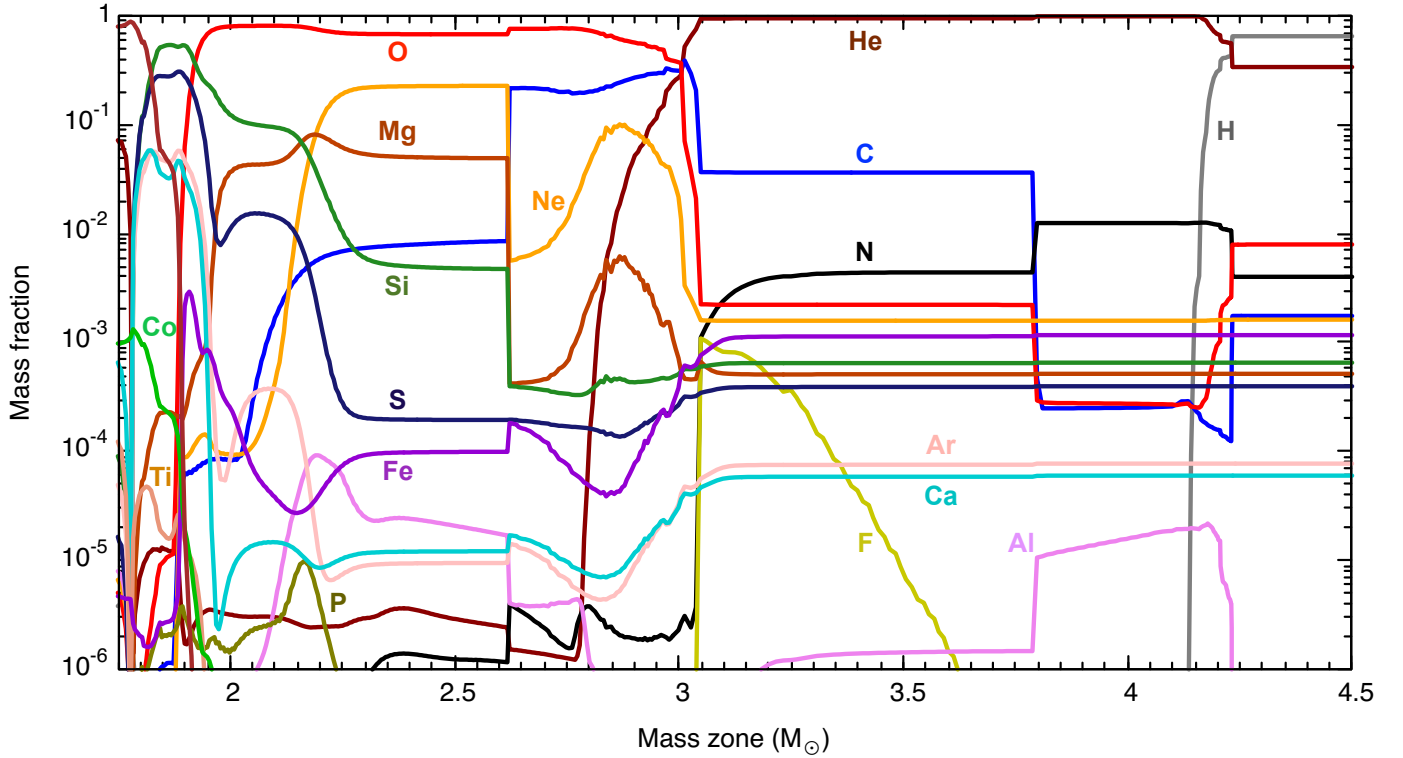


Fig. 1. Elemental composition as a function of enclosed mass for a Type II-P SN with $15 M_{\odot}$ progenitor as modelled by Rauscher et al. (2002), model s15a27c, with explosion kinetic energy of 1.2B.

from the centre at the reference time t_0 , and E_i^{γ} is the energy emitted per decay in γ -rays. For each isotope, $\tau_{i,0}$ is defined as (Woodsley et al. 1989; Cherchneff & Dwek 2009):

$$\tau_{i,0} = \kappa_i \frac{3 M_{\text{He}}}{4\pi r(t_0)^2} \quad (5)$$

where M_{He} is the mass of the helium core, κ_i is the average γ -ray mass absorption coefficient, and $r(t_0)$ is the radius of the ejecta at time, t_0 .

Owing to the rapid decay of ^{56}Ni and ^{57}Ni compared to the ejecta dynamical time, we assume $M(^{56}\text{Co}) = M(^{56}\text{Ni})$ and $M(^{57}\text{Co}) = M(^{57}\text{Ni})$. Similarly, we take $M(^{44}\text{Ca}) = M(^{44}\text{Ti})$. The relevant parameters for the decay chains we consider and the calculation of the energy deposition rate as given by Equation (4) are summarised in Table 1. We chose $t_0 = 100$ days post-explosion as a reference time to start our calculations, leading to the following energy deposition rates as a function of time t , in ergs s^{-1} , expressed as

$$L_{^{56}\text{Co}}(t) = 1.61857 \times 10^{42} \times e^{-(t/111.43)} \times [1 - e^{-17.17(t/100)^{-2}}], \quad (6)$$

$$L_{^{57}\text{Co}}(t) = 5.08965 \times 10^{38} \times e^{-(t/392.04)} \times [1 - e^{-41.21(t/100)^{-2}}], \quad (7)$$

$$L_{^{44}\text{Ti}}(t) = 1.26241 \times 10^{36} \times e^{-(t/31121.10)} \times [1 - e^{-20.81(t/100)^{-2}}]. \quad (8)$$

The total γ -ray-energy deposition rate to be considered in the calculation of the ionisation rates by Compton electrons is then

$$L_{\text{tot}}(t) = L_{^{56}\text{Co}}(t) + L_{^{57}\text{Co}}(t) + L_{^{44}\text{Ti}}(t). \quad (9)$$

The elemental composition after explosion of the s15a27c model by Rauscher et al. (2002) is represented in Fig. 1. In this model, the entire ejecta, defined by Truelove & McKee (1999) as the core and the envelope, has a mass of $M_{\text{ej}} = 12.61 M_{\odot}$,

whereas the helium-rich (hereafter He-rich) ejecta core mass is $4.23 M_{\odot}$. For the purpose of this study, focussed on the synthesis of molecules and dust clusters, we consider the matter comprised between the mass zones $1.78 M_{\odot}$ and $4.14 M_{\odot}$ in Fig. 1; namely, $2.36 M_{\odot}$ of He-rich and hydrogen-free ejected gas, represented by 332 zones, each zone having a specific velocity and being of variable mass in the range $5 \times 10^{-3} - 1.35 \times 10^{-2} M_{\odot}$. As previously mentioned, we assumed a spherically symmetric ejecta whose elemental composition remains stratified after the star has exploded, despite the existence of Rayleigh-Taylor instabilities and macroscopic mixing within the He core triggered by the reverse shock at the base of the hydrogen envelope.

To facilitate the comparison with molecular lines and dust observations, we assigned a velocity for each mass zone following the description of Truelove & McKee (1999), which was later used by Sarangi (2022) for his model of SN1987A. According to Truelove & McKee (1999), the ejecta follows homologous expansion ($r_{\text{ej}} \propto t$, where r_{ej} is the ejecta radius) and is made of a uniform core and an envelope with a density profile of $\rho_{\text{en}} \propto r^{-n}$, where $n \simeq 12$ in case the progenitor is a red supergiant (RSG, Matzner & McKee 1999). Truelove & McKee derived a velocity, v_c , at the core-envelope interface in the limit of $w_{\text{core}} = v_c/v_{\text{ej}} \rightarrow 0$, where v_{ej} is the velocity of the ejecta at the ejecta-ambient medium interface, given by

$$v_c = \sqrt{\frac{10(n-5) E_{\text{ex}}}{3(n-3) M_{\text{ej}}}}, \quad (10)$$

where E_{ex} is the explosion energy. According to the authors, the density of the ejecta core is given by

$$\rho_c = \frac{3}{4\pi} \frac{n-3}{n} \frac{M_{\text{ej}}}{(v_c t)^3}. \quad (11)$$

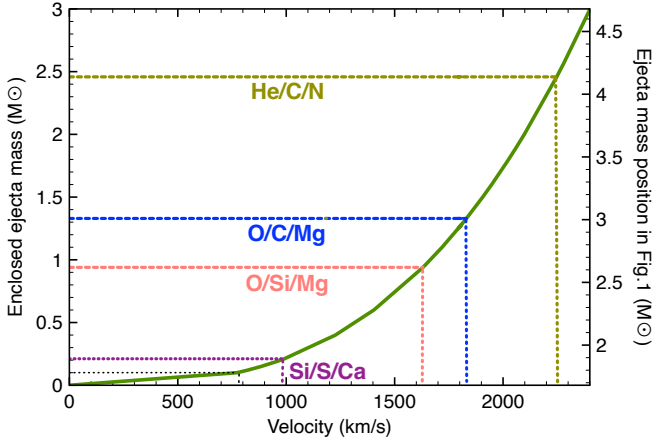


Fig. 2. Zone velocity as a function of enclosed mass and zone position for the $15 M_{\odot}$ explosion model of Rauscher et al. (2002).

The enclosed mass, M_{enc} , is the mass comprised under a certain mass zone in the ejecta, given by

$$M_{\text{enc}} = \frac{4\pi}{3} \rho_c (vt)^3, \quad (12)$$

where v is the zone velocity. By combining Equations (10), (11), and (12), we derive the following expression for the velocity as a function of enclosed mass, thereby translating zone position into zone velocity in the ejecta,

$$v = \frac{n}{n-3} \left[\frac{M_{\text{enc}}}{M_{\text{ej}}} \right]^{1/3} \times v_c. \quad (13)$$

The necessary parameters are listed in Table 1. The zone position-velocity correspondance is shown in Fig. 2.

From the perspective of a chemical study of the ejecta, we organised the 332 mass zones in different regions, according to the chemical composition and the dominant elemental species present in each region following Kozma & Fransson (1998), Cherchneff & Lilly (2008), Cherchneff & Dwek (2009), and Sarangi & Cherchneff (2013). However, instead of deriving an averaged elemental composition for each region to study the chemistry (see Cherchneff & Dwek 2009; Sarangi & Cherchneff 2013), here we investigated the chemistry of each specific zone included in a region and summed over all the zones to derive important quantities such as the molecule and dust cluster masses. There are four major regions in total that cover the ejecta, whose parameters are listed in Table 2.

2.2. Gas density

We study the time evolution of the entire ejecta by following the time evolution of the chemistry in each zone of the stratified ejecta at a starting time $t_0 = 100$ days. Each zone expands with time at a certain velocity given by Equation (13) and follows homologous expansion so that the gas number density varies with time according to the equation,

$$n_{\text{gas}}(M_r, t) = \rho_{\text{gas}}(M_r, t_0) / \mu(M_r, t_0) \times (t/t_0)^{-3}, \quad (14)$$

where $\rho_{\text{gas}}(M_r, t_0)$ and $\mu(M_r, t_0)$ are the gas density and the mean molecular weight at $t_0 = 100$ days, respectively, in the mass zone of coordinate M_r . In their study of Type IIP SNe, Utrobin et al. (2017) modelled the light curve of a typical $15 M_{\odot}$ progenitor and derive gas densities for the ejecta out of three-dimensional

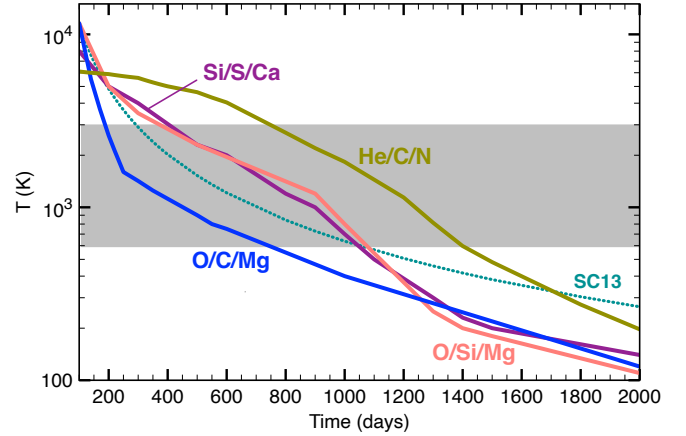


Fig. 3. Gas temperature for the ejecta regions defined in Table 2 as a function of the post-explosion time from Kozma & Fransson (1998), except the O/C/Mg zone where values are from Liljegren et al. (2020). The label SC13 refers to the temperature profile used in Sarangi & Cherchneff (2013). The shaded area represents the temperature regime at which dust forms in dust-producing experiments in the laboratory (e.g. high-temperature flame or vapour condensation experiments).

(3D) simulations of neutrino-driven explosions. The gas density profiles, as a function of interior mass, were averaged over different angular directions, resulting in a fairly constant gas density over the mass zone range $2.2\text{--}5 M_{\odot}$ at $t_{\text{ex}} = 1.29$ days, with $\rho_{\text{gas}}(M_r, t_{\text{ex}}) \sim 1 \times 10^{-7} \text{ g/cm}^{-3}$.

For the sake of simplicity, we assumed a constant gas density over the ejecta core and chose the average value derived by Utrobin et al. (2017) at the position $M_r = 2.1 M_{\odot}$. At t_{ex} , we have $\rho_{\text{gas}}(2.1, t_{\text{ex}}) = 6.3 \times 10^{-8} \text{ g/cm}^{-3}$. Assuming a t^{-3} expansion, the gas density at t_0 is then equal to $1.35 \times 10^{-13} \text{ g/cm}^{-3}$ for the mass zones comprised between $1.78 M_{\odot}$ and $4.14 M_{\odot}$. This gas density value is very close to that derived from Equation 11 ($\rho_c(t_0) = 1.59 \times 10^{-13} \text{ cm}^{-3}$) and characterises our standard case for this study. The zone number densities at t_0 calculated from Equation (14) are consistent with values derived from the analysis of SN light curves (e.g. SN1987A).

2.3. Gas temperature

The temperatures for the various ejecta regions are displayed in Fig. 3, along with the temperature variation that was used in Sarangi & Cherchneff (2013). These temperatures were derived for the ejecta of SN1987A by Kozma & Fransson (1998), who modelled all thermal and non-thermal heating and cooling processes in the ejecta as a function of time. In the four regions shown in Table 2, which have different elemental compositions, the temperature profiles drastically vary from one another when going from the inner region outwards. For example, the inner regions are rich in heavy elements compared to the outer carbon-rich region and, thus, they cool faster through atomic line emissions. In contrast, the He/C/N region will remain hot over the period day 100–1000 as seen in Fig. 3.

A special case is represented by the region O/C/Mg, which produces most of the CO molecules, as shown by Liu et al. (1992), Cherchneff & Dwek (2009), and Sarangi & Cherchneff (2013). The strong cooling resulting from the collision-induced vibrational emission of CO forces the gas temperatures to sharply drop before day 500 so that the region is much cooler

Table 2. Parameters of regions in the stratified ejecta with 15 M_⊙ progenitor (Rauscher et al. 2002).

Region	Si/S/Ca	O/Si/Mg	O/C/Mg	He/C/N	Ejecta
Major elements	Si–S–Ca–Ar	O–Si–Mg–Ne	O–C–Ne–Mg	He–C–N–O	
Boundaries ^a	1.783–1.894	1.894–2.623	2.623–3.013	3.013–4.141	
Velocity range ^b	774–990	991–1630	1631–1830	1831–2247	
Number of zones	22	145	70	95	332
Mass ^a	0.111	0.729	0.390	1.128	2.358

Notes. ^(a) in M_⊙, ^(b) in km s⁻¹.

than others (Liu et al. 1992; Liljegren et al. 2020). We actually chose the temperature profile derived by Liljegren et al. (2020) for our model. As pointed out by Liu & Dalgarno (1995), any of the ejecta regions that forms molecules in relevant quantities experiences strong molecular cooling. This is true for the O/Si/Mg region, which forms large amounts of SiO and for which a gas temperature profile lower than the one shown in Fig. 3 could also be considered.

The ejecta temperatures were modelled for SN1987A, which has a progenitor of ~19 M_⊙ and injected ~0.075 M_⊙ of ⁵⁶Ni in the ejecta. Our SN template has slightly different parameters as seen from Table 1. Since, to date, there is no temperature model available for such a progenitor, we adopted the profiles for SN1987A, while assuming the temperature trends of the ejecta regions hold for other progenitor (specifically, the molecular cooling in molecule-forming regions and the high temperature of the outer ejecta region). The temperature profile of each region as a function of time is fitted by a sum of power laws in order to be implemented within the code.

3. The chemical model

Modelling the chemistry active in the ejecta requires setting up a list of relevant species and molecules, including neutrals and ions. Some species have already been observed in SNe, while others are closely linked to them chemistry-wise. We also considered molecular species that are observed in other astrophysical environments (e.g. the wind of low- and high-mass evolved stars) or planetary atmospheres. Overall, we ought to bear in mind that with the He core of the SN ejecta being H-free, this condition restricts our choice of species and related chemical processes. As for dust clusters, we considered several groups of solids identified in pre-solar grains of SN origin and their molecular precursors. These solids include silicates, silica, alumina, carbon, silicon carbide, and silicon nitride (Hoppe et al. 2022).

3.1. Method

We considered formation pathways identified in the laboratory or proposed on the basis of established chemical structures and exo/endothemicity of reaction processes. All species we considered are gathered in Table 3. We included 203 chemical species and 1447 reactions in total, which reaction rates are documented or estimated. Most of them are taken from the following chemical databases: National Institute of Standards and Technology Chemical Kinetics Database (Manion et al. 2008), UMIST22 (Millar et al. 2024), and KIDA (Wakelam et al. 2024). For non-documented rates, the estimation is based on the calculation of reaction energies that are chosen as activation barriers for endothermic processes. The set of reactions consists of thermal

and non-thermal processes, which description and occurrence regime are gathered in Table A.1 of the Appendix.

The temporal variation of the number density, n , of a molecular species, i , located at a given mass zone, z , is described by the following rate equation,

$$\begin{aligned} \frac{dn_i(z, t)}{dt} &= P_i - L_i \\ &= \sum_j k_{ji}(t)n_j(z, t)n_i(z, t) - \sum_k k_{ik}(t)n_i(z, t)n_k(z, t), \end{aligned} \quad (15)$$

where P_i and L_i are the production (\equiv formation) and loss (\equiv destruction) term, respectively, and k_{ji} is the reaction rate coefficient for a reaction between species j and i . The reaction rate is provided in a Arrhenius form as follows,

$$k_{ij}(t) = A_{ij} \left[\frac{T(t)}{300} \right]^n \exp(-E_a/T(t)), \quad (16)$$

where T is the gas temperature, A_{ij} the Arrhenius coefficient (in s⁻¹ molecule⁻¹, cm³ s⁻¹ molecule⁻¹, and cm⁶ s⁻¹ molecule⁻¹ for a unimolecular, bimolecular, and termolecular process, respectively), n reflects the temperature dependence of the reaction, and E_a is the activation energy barrier along the reaction path.

The destruction rate by Compton electrons of species, i , leading to ionisation or dissociation (Cherchneff & Dwek 2009) is defined as

$$k_{C,i}(t) = \alpha \frac{L_{\text{tot}}(t)}{N_{\text{tot}}W_i}, \quad (17)$$

where $L_{\text{tot}}(t)$ is the total deposition rate for γ -rays as given by Equation (4), N_{tot} is the total number of ejecta particles, and α is the fraction of the deposited energy in the ejecta that goes into ionisation and dissociation of atoms and molecules. For SN1987A, values for α as a function of post-explosion time were calculated in the range 0.2–0.4 in the various core zones by Kozma & Fransson (1992). A value of ~0.38 was derived by Liu & Dalgarno (1995) for a ionisation fraction of 2×10^{-2} . We chose $\alpha \sim 0.35$ as used in previous physico-chemical models of SN ejecta (Sluder et al. 2018; Sarangi 2022). Finally, W_i is the mean energy per ion-pair for species i (in eV), and is defined as the ratio of the energy of the incident electron divided by the number of ionisation or dissociation produced by collision with the incident electron until it comes to rest (Liu & Dalgarno 1994; Dalgarno et al. 1999). Values of W_i are taken from Cherchneff & Dwek (2009). In the present model, we do not consider the freeze-out of ionisation within the ejecta after day 800 as evidenced by Fransson & Kozma (1993). At late epochs, the ionisation fraction is already low ($x < 10^{-3}$) and we do not expect the freeze-out of ionisation to affect our results.

Modelling the chemistry of the ejecta consists of solving 203 stiff, coupled, ordinary differential equations as described

by Equation (15) for each mass zone and the gas conditions described in Sects. 2.2 and 2.3. We first chose a few mass zone positions for each ejecta region and specifically study the chemistry active at these positions to identify the chemical processes at the origin of molecule and dust cluster formation. Thus, we derived the number densities and mass fractions for the 203 species as a function of post-explosion time and identified prominent species formed at specific positions in the ejecta. Secondly, we ran the chemistry for each zone across the ejecta regions and sum up the masses of species we obtain to derive the total mass of species produced per ejecta region as a function of time. Finally, we summed the masses obtained per region for each species to derive the variation of the final mass formed as a function of time across the ejecta. This method provides an exhaustive grasp of the chemistry taking place across the ejecta and the evolution of the mass budget of molecules and dust clusters with post-explosion time.

One major improvement of this study resides in considering one unique chemical scheme applied to all ejecta regions. Previous studies assume each region is governed by its own chemistry and chemical scheme in line with the initial elemental composition of the region (e.g. Cherchneff & Dwek 2009; Sarangi & Cherchneff 2013), and this type of assumption is adopted in recent studies (Sarangi 2022; Sarangi et al. 2025). This restriction on the chemistry at play induces a biased outlook on what an ejecta region might produce by limiting the various types of species formed in each region; for example, the exclusion of the formation of oxides in carbon-rich regions and C-bearing molecules in O-rich zones.

We briefly discuss below our choices of species, dust molecular clusters, and the new chemical pathways leading to the formation of silicate, silica, alumina, and carbon dust clusters.

3.2. Silicates and silica

The nucleation of silicate clusters remains an enigma, both experimentally and theoretically. The condensation of Mg-SiO-H₂-O₂ vapours results in the formation of magnesosilica smoke where grains are arranged in necklaces and agglomerates. MgO (periclase) and SiO₂ (silica) inclusions are also found in these grains of stoichiometric enstatite (MgSiO₃) or forsterite (Mg₂SiO₄) chemical composition (Rietmeijer et al. 2002). Flash-evaporation experiments exploiting the vapour phase from magnesium and silicon oxide in a mixed atmosphere of Ar and O₂ to form silicates, show the grains change from crystalline to amorphous as the Mg-to-Si ratio decreases (Kimura et al. 2008).

The natural precursor to silicates in circumstellar environments is the molecule SiO, which is abundant in the wind of AGB and supergiants stars, and SN ejecta. Theoretical studies have focussed on identifying chemical structures of relevant clusters and routes linking SiO, SiO dimers and silicate molecular clusters. For example, Escatllar et al. (2019) employ global-optimisation methods to find the lowest-energy isomers of (MgSiO₃)_N and (Mg₂SiO₄)_N clusters for N = 1 – 10. Interestingly, the MgSiO₃ and Mg₂SiO₄ monomers are both kite-shaped with one external O atom, and are thus reactive molecules. In the context of understanding dust formation in the H-rich wind of AGB stars, Goumans & Bromley (2012) derive exothermic chemical pathways consisting of the dimerisation of SiO as a bottleneck to the formation of Si₂O₃, followed by the addition of Mg atoms to form small molecular clusters of the type Mg_xSi_yO_z with silicate stoichiometry. These pathways are adopted by Sarangi & Cherchneff (2013) for a H-free gas

and used to model the formation of silicate clusters in several SN environments (Sarangi & Cherchneff 2015; Sluder et al. 2018; Sarangi 2022; Sarangi & Slavin 2022; Sarangi et al. 2025; Purushothaman et al. 2025).

However, a quantum chemical study of SiO clustering by Bromley et al. (2016) shows the dimerisation is too slow a process under the physical conditions (i.e. gas temperature and pressure) found in circumstellar environments to induce silicate nucleation. Experimental investigations on SiO clustering from vapour, which show very inefficient grain formation, also corroborate the finding that SiO dimerisation is inefficient at triggering the formation of silicate clusters (Kimura et al. 2022). Therefore, both theoretical and experimental studies invalidate the chemical model used so far for the synthesis of silicates in SNe and question the reliability of the results on dust by existing investigations.

To revisit the problem of silicate nucleation, we explore new chemical pathways based on the initial conditions met in a SN ejecta, which we consider H-free, and rich in Mg, O, and Si, like the region O/Si/Mg of Table 2. The formation of dust is observed in many SN ejecta characterised by various stellar progenitor masses, explosion energies, and physical conditions. We thus wish to identify a simple chemical scheme efficient enough to sustain dust formation under different SN environments. Starting with simple di- and triatomic molecules we find are abundant in the ejecta gas (e.g. SiO, MgO, SiO₂ and MgO₂), we pinpoint all possible exothermic and some slightly endothermic chemical channels that buildup small intermediate clusters Mg_xSi_yO_z with $x = 0-4$, $y = 0-1$ and $z = 1-4$. We characterise these small silicate molecular clusters by deriving stable structures from density functional theory (DFT) and follow their chemical growth to finally form MgSiO₃ and Mg₂SiO₄ molecules and their dimers.

The exo- or endothermicity of a reaction is calculated by deriving the reaction energy ΔE given by

$$\Delta E = \sum_{\text{products}} E - \sum_{\text{reactants}} E, \quad (18)$$

where E is the absolute energy of a species at 0 K and includes zero-point corrections. Energy data on small silica are from Lu et al. (2003) while we calculate from DFT the energies for silicate intermediates. For a few silicate clusters, we use existing values from Goumans & Bromley (2012). All calculations are made at the B3LYP/6-31G(d) level. The relevant new chemical reactions leading to the formation of MgSiO₃ and Mg₂SiO₄ monomers and dimers are listed in Table 4 along with their reaction energy, whereas the calculated absolute energies at 0 K of the silicate molecular clusters used in our chemical description are listed in Table A.2 of the Appendix.

Existing chemical models consider that the formation of silica (SiO₂) occurs as a consequence of the polymerisation of SiO to form (SiO)_n clusters. The polymerisation is followed by silicon segregation and formation of SiO₂ units in silicon monoxide clusters as the clusters size increases, usually for $n > 10$ (Wang et al. 2008; Reber et al. 2008). As we mentioned previously, the polymerisation of SiO is extremely inefficient at forming clusters for circumstellar gas conditions. This implies the synthesis of silica clusters must operate through other channels. Therefore, we investigate the formation of small silica clusters up to (SiO₂)₃ \equiv Si₃O₆ by considering all exothermic reactions leading to the formation of the trimer and taking into account the structures as provided by Lu et al. (2003). These chemical pathways mainly involve the exothermic reaction SiO₂ + SiO₂ \rightarrow Si₂O₃ + Si to form Si₂O₃ and subsequent

Table 3. Atoms, molecules, ions, and dust molecular clusters considered in the new chemical model.

Atoms and molecules								
O	O ₂	O ₃	OF	MgO	AlO	SiO	PO	SO
C	C ₂	C ₃	CN	CO	CO ₂	CF	CP	CS
Si	Si ₂	SiC	SiN	SiO ₂	SiO ₃	SiP	SiS	
N	N ₂	NO	NO ₂	NF	NS			
S	S ₂	CS ₂	SO ₂	OCS				
Mg	Mg ₂	MgO ₂	MgS	MgS ₂				
Al	Al ₂	AlO ₂	AlO ₃	Al ₂ O				
Ca	Ca ₂	CaO	CaO ₂	CaS	CaS ₂			
Fe	Fe ₂	FeO	FeO ₂	FeO ₃	FeS			
P	P ₂	PN	PO ₂	PS	PS ₂			
F	F ₂	MgF	AlF	SiF	CaF			
He	Ne	Ar	⁴⁴ Ti	⁵⁶ Co	⁵⁶ Ni			
Atomic and molecular ions								
O ⁺	O ₂ ⁺	MgO ⁺	AlO ⁺	OCS ⁺				
C ⁺	C ₂ ⁺	C ₃ ⁺	CN ⁺	CO ⁺	CO ₂ ⁺	CS ⁺		
Si ⁺	SiC ⁺	SiN ⁺	SiO ⁺	SiS ⁺				
N ⁺	N ₂ ⁺	NO ⁺	NO ₂ ⁺	NS ⁺				
S ⁺	SO ⁺	SO ₂ ⁺						
Al ⁺	AlO ₂ ⁺							
Ca ⁺	CaO ⁺							
Fe ⁺	FeO ⁺	FeO ₂ ⁺	FeS ⁺					
P ⁺	PO ⁺							
Mg ⁺	F ⁺	He ⁺	Ne ⁺	Ar ⁺				
Dust clusters and ions								
(Mg) _{n=3,6}	(MgO) _{n=2,4}	(MgS) _{n=2,4}	(Fe) _{n=3,6}	(FeO) _{n=2,4}	(FeS) _{n=2,4}	(SiO) _{n=2,20}	(CaO) _{n=2,4}	(CaS) _{n=2,4}
Al ₂ O ₂	Al ₂ O ₃	Al ₂ O ₄	Al ₃ O ₃	Al ₄ O ₆	Si ₂ O ₃	Si ₃ O ₄	Si ₃ O ₅	Si ₃ O ₆
MgSiO	MgSiO ₂	MgSiO ₃	Mg ₂ SiO ₂	Mg ₂ SiO ₃	Mg ₂ SiO ₄	Mg ₂ Si ₂ O ₆	Mg ₄ Si ₂ O ₈	
(C) _{n=4,20}	(C) _{n=4,10} ⁺							

exothermic reactions with SiO₂ to grow to Si₃O₅ and SiO₂ trimers.

3.3. Alumina

The structure of Al₂O₃ clusters (Al₂O₃)_{N=1,7} were studied by Li & Cheng (2012) while structures of aluminum oxide (Al_{n=2,7}O_{m=1,10}) clusters were extensively investigated by Armstrong et al. (2019). When the Al₂O₃ unit has a kite-shaped structure, the dimer (Al₂O₃)₂ is a cage. However, cage structures become unstable with increasing cluster sizes and disordered structures are favourable for large clusters. A recent study by Saba et al. (2021) explores the gas-phase synthesis of alumina from aluminium oxidation. Based on DFT, they construct a detailed chemical kinetic description of alumina formation in a O₂ environment. In the present model, we stop our cluster growth at the formation of alumina dimers (≡ Al₄O₆) and base our chemical description on results from Saba et al. (2021), Swihart & Catoire (2000), and Glorian et al. (2016).

3.4. Carbon clusters

The formation of pure (≡ H-free) carbon clusters was extensively studied 30 years ago after the discovery of the Buckminsterfullerene cage molecule, C₆₀ (Kroto et al. 1985). Since then, a consensus was reached in nano-science on the formation of pure carbon cages, which involves the growth of small carbon chains up to C₉ into carbon single or multiple rings and open cages, the smallest cage identified in the laboratory being C₂₈. The growth

of cage lattices occurs through the incorporation of atomic C and C₂ (Dunk et al. 2012). The structure of small carbon chains and rings is then important to better model the formation of carbon grains in circumstellar environments.

In this study, we revisit and improve the formation processes of carbon chains and rings up to C₂₀. Following Remya & Suresh (2016), we consider that carbon clusters are chains for C₂₋₅ and C₇₋₉ and rings for C₆ and C₁₀. The chemistry of small carbon clusters up to C₁₀ is that of Loison et al. (2014) for reactions between small chains and Clayton et al. (1999) for radiative association processes. For reaction of C₂ with small chains (≡ C_n with n = 3–7), we use DFT to derive energy budgets along the reaction path and assess exo/endothemicity and barriers. We further describe the growth of rings through C incorporation taking into account the ring opening energies derived by Remya & Suresh (2016), while our description of ring growth through C₂ addition is based on the study by Schweigert et al. (1995). The dimerisation of C₆ and C₁₀ described by Remya & Suresh (2016) is also considered. We believe this new description provides more accurate formation pathways for carbon clusters up to C₂₀ at the high- and low-gas temperatures met in the ejecta.

3.5. Other clusters

On top of silicate, silica, alumina, and carbon clusters, we modelled the formation of silicon diatomic Si₂ and sulphur diatomic S₂ species as potential first-step products in the formation process of pure Si and S solids. For iron, we modelled the formation

Table 4. Reactions for the nucleation of silicate dimers.

	Reactants		Products		ΔE^a
R1	MgO	+ MgO	→ MgO ₂	+ O	-86.4
R2	MgO	+ SiO	→ SiO ₂	+ Mg	-188.3
R3	MgO	+ SiO ₂	→ SiO ₃	+ Mg	-16.3
R4	MgO ₂	+ SiO	→ SiO ₃	+ Mg	-98.1
R5	MgO ₂	+ SiO ₂	→ MgSiO ₃	+ O	-263.4
R6	MgSiO ₃	+ MgO ₂	→ Mg ₂ SiO ₄	+ O	-269.1
R7	MgO	+ SiO ₂	→ MgSiO	+ O ₂	+54.3
R8	MgO	+ SiO ₃	→ MgSiO ₃	+ O	-342.3
R9	Mg ₂ O ₂	+ SiO ₃	→ Mg ₂ SiO ₄	+ O	-355.3
R10	MgO ₂	+ SiO	→ MgSiO ₂	+ O	-377.9
R11	MgSiO ₂	+ MgO	→ MgSiO ₃	+ Mg	-291.2
R12	MgSiO ₂	+ O ₂	→ MgSiO ₃	+ O	+41.8
R13	MgO ₂	+ SiO	→ MgSiO	+ O ₂	-32.1
R14	MgSiO	+ O ₂	→ MgSiO ₂	+ O	-128.5
R15	MgSiO ₂	+ MgO	→ Mg ₂ SiO ₂	+ O	+73.5
R16	MgSiO ₂	+ MgO ₂	→ Mg ₂ SiO ₂	+ O ₂	-147.5
R17	Mg ₂ SiO ₂	+ MgO ₂	→ Mg ₂ SiO ₄	+ Mg	-663.7
R18	Mg ₂ SiO ₂	+ O ₂	→ Mg ₂ SiO ₃	+ O	-90.5
R19	MgSiO ₂	+ MgO ₂	→ Mg ₂ SiO ₃	+ O	-237.1
R20	Mg ₂ SiO ₃	+ MgO ₂	→ Mg ₂ SiO ₄	+ Mg	-323.1
R21	Mg ₂ SiO ₃	+ O ₂	→ Mg ₂ SiO ₄	+ O	-2.2
R22	MgSiO ₃	+ MgSiO ₃	→ Mg ₂ Si ₂ O ₆		-770.3
R23	Mg ₂ SiO ₄	+ Mg ₂ SiO ₄	→ Mg ₄ Si ₂ O ₈		-2407.5

Notes. ^(a) Reaction energy in kJ mol⁻¹.

of small (Fe)_{n=2,6} clusters based on a study of iron nanoparticle synthesis by condensation of iron vapour at temperatures of ~1000 K (Giesen et al. 2003). A complementary study by Wen et al. (2007), who derived detailed chemical kinetic models for gas-phase synthesis of iron nanoparticles, was also used. Finally, we considered the formation of metal sulphide solids by including the polymerisation of small (MgS)_{n=2,4}, (CaS)_{n=2,4} and (FeS)_{n=2,4} clusters, for which we adopted the rates derived for (SiO)_n polymerisation (Bromley et al. 2016).

We did not model the formation of small silicon carbide, SiC, and silicon nitride, Si₃N₄, clusters at this stage but included formation processes for the two parent molecules SiC and SiN to better understand where these molecular precursors form in the ejecta.

3.6. Phosphorous and fluorine

We see from Fig. 1 that phosphorous, P, is present in the inner O/Si/Mg region, while the mass fraction of fluorine, F, is important in the inner part of the He/C/N region. Phosphorous molecules were detected in the H-rich circumstellar environments of evolved stars. Phosphorous monoxide PO, was first detected in the wind of the supergiant star VY Cam (Tenenbaum et al. 2007) while both PO and PN were observed in the wind of the O-rich AGB star IK Tau (De Beck et al. 2013). Finally, carbon and silicon monophosphide, CP and SiP respectively, were both identified in the wind of the carbon star IRC+10216 (Guelin et al. 1990; Koelmay et al. 2022). As for fluorine, AIF was observed again in the wind of IRC10216 at millimetre wavelengths (Cernicharo & Guelin 1987; Ziurys et al. 1994), but the search for MgF and CaF was unfruitful.

To assess whether SN ejecta produce P- and F-bearing molecules, we include in our new chemical scheme the fluoride and phosphide species listed in Table 3 and the related chemistry.

4. Results

With the purpose of identifying the chemical processes controlling the synthesis of molecules and dust clusters, we studied the ejecta by first considering a standard case, defined as follows: (1) the gas number density is derived from the initial density at day 100, as given in Table 1; and (2) the gas temperatures in the various ejecta regions are those illustrated in Fig. 3. For each ejecta region, we present our results on molecule and cluster mass fractions versus post-explosion time at a specific zone position to discuss the chemistry at play. We provide the total masses of molecules and dust clusters formed over the entire region as well as mass maps. Results for the Si/S/Ca region are presented in Sect. 4.1, while the results for the O/Si/Mg, O/C/Mg, and He/C/N regions are presented in Sects. 4.2, 4.3, and 4.4, respectively.

We then considered two cases out of our standard case to investigate two specific issues: (1) a high-density case for the He/C/N region to study the conditions required for the efficient nucleation of carbon dust clusters; and (2) a low-temperature profile for the O/Si/Mg region to assess the impact of lower temperatures on the synthesis of silicates, silica and alumina. Results for the high-density case are presented in Sect. 4.5, while those for the low-temperature case are summarised in Sect. 4.6.

Finally, all molecular and cluster mass values for the entire ejecta and the standard case are gathered in Table 5.

4.1. The Si/S/Ca region

In this region, we chose the zone position $z = 1.85 M_{\odot}$ to investigate the chemistry since the mass fraction of oxygen is still small. As seen from Fig. 4, the prominent molecules are SiS, CaS, FeS, and MgS and they readily form. The dominant formation pathways for these molecules are through reaction with S₂ and radiative association as follows



The rate for reaction (19) has not yet been studied while reaction of C with S₂ to form CS is well documented (Mitchell 1984; Smith et al. 2004). As in Cherchneff & Dwek (2009), we use the isovalence of Si and C to attribute a rate to reaction (19). A similar approach is used to estimate the rate for reaction (21) by assuming isovalence of O and S and the rate of FeO formation (Smirnov 2012). Likewise, we use the isovalence of O and S, and Mg and Ca, for determining the rates of reactions (20) and (22), since the radiative association reaction between Mg and O is studied by Bai et al. (2021).

Because the reaction rates for the dominant formation processes of these four molecules are estimated, we want to test whether their high mass fractions are sensitive to our choice of rates. We decrease by a factor of 100 the rates and obtain unchanged results for the SiS, CaS, FeS, and MgS mass fractions. The robustness of these results is due to the combination of the limited chemistry controlling the Si/S/Ca region compared to other ejecta regions, and the initial elemental composition that lacks oxygen.

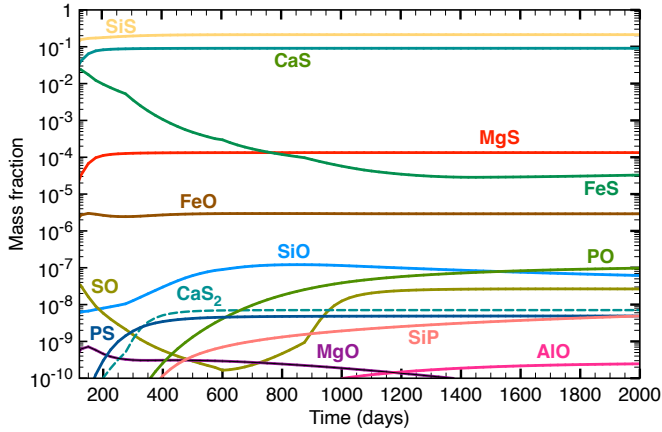


Fig. 4. Mass fractions of molecules produced in the Si/S/Ca ejecta region at $z = 1.85 M_{\odot}$ as a function of post-explosion time for the standard case. The zone mass is $4.64 \times 10^{-3} M_{\odot}$.

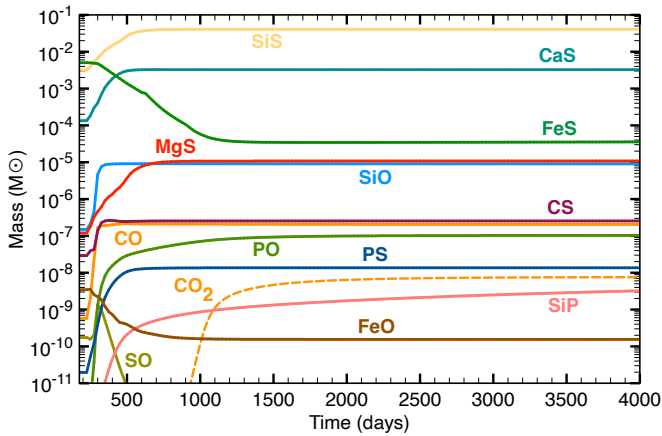


Fig. 5. Total masses of molecules produced over the Si/S/Ca region as a function of post-explosion time for the standard case. The region mass is $0.111 M_{\odot}$ (see Table 2).

The prominent molecules formed over the entire Si/S/Ca region are SiS and CaS, and to a lesser extent, FeS and MgS, as seen from Fig. 5 where the total molecular masses summed over the Si/S/Ca region are presented as a function of post-explosion time. Towards the outer part of the region where the oxygen mass fraction starts rising (see Fig. 1), some O-bearing species form in small quantities (e.g. SiO and PO). While the molecular budget represents $\sim 39.7\%$ of the region's mass, none of the dust clusters present in our model are synthesised in relevant quantities in this region.

4.2. The O/Si/Mg region (Inner oxygen region)

The O/Si/Mg region contains mostly atomic oxygen and high mass fractions of atomic silicon, magnesium, and sulphur (see Fig. 1). Therefore, this region forms most of the silicate, silica, and alumina clusters in the ejecta. As mentioned in Sect. 3.6, phosphorous is also present, although in much lesser quantities. A significant mass fraction of Ne characterises this region but it remains always smaller than that of atomic oxygen. Compton electrons ionise Ne to create a population of Ne^+ ions that dissociates molecules and returns to the neutral state. However, it is prominently molecules like O_2 that drive the chemistry of the

region. The situation is drastically different in the He/C/N region where He^+ controls the time of molecular formation.

4.2.1. Results for $z = 2.15 M_{\odot}$

We present results for the zone position $z = 2.15 M_{\odot}$, which shows high O, Si, and Mg initial mass fractions, as well as a P maximal initial mass fraction. The position has thus optimal conditions to conduce to silicate formation and results are shown for molecules in Fig. 6 and dust clusters in Fig. 7. We see in Fig. 6 that O is over-abundant at early times so that O_2 forms according the radiative association,



The formation of O_2 continues mainly through the reaction,



and to a lesser extent,



while the reverse processes provide the prominent destruction routes. When the gas temperatures drops below ~ 3500 K, molecular formation is boosted over a 40 day time-span at \sim day 300, with O_2 capturing most of atomic O and controlling the molecular phase. Assuming that the chemistry operates as described herein, caution should then be exercised in the use of atomic oxygen masses as a supernova diagnostic.

The rapid conversion of atomic O into O_2 results in the efficient formation of molecules like SiO, SO_2 , CO_2 , and CO from oxidation reactions of atomic species such as Si or C with O_2 . For example, SO forms out of



but is efficiently destroyed by its conversion into SO_2 through



Interestingly, PO and PO_2 are the only abundant P-bearing species before day 1000 experiencing similar formation processes,



and

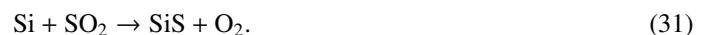


While reaction (28) is slightly exothermic, reaction (29) is slightly endothermic and, thus, it proceeds at high gas temperatures. The reaction stops at around day 1000 when the gas temperature drops below ~ 800 K, resulting in a decrease in PO_2 mass fraction.

Finally, some MgS, SiS, and CaS form at this position, albeit in smaller quantities. While MgS and CaS form out of radiative association over the entire time-span, SiS formation relates to SiO and SO_2 through



and



As for dust clusters, inspection of Fig. 7 reveals the efficient synthesis of silicates through various intermediates as soon as

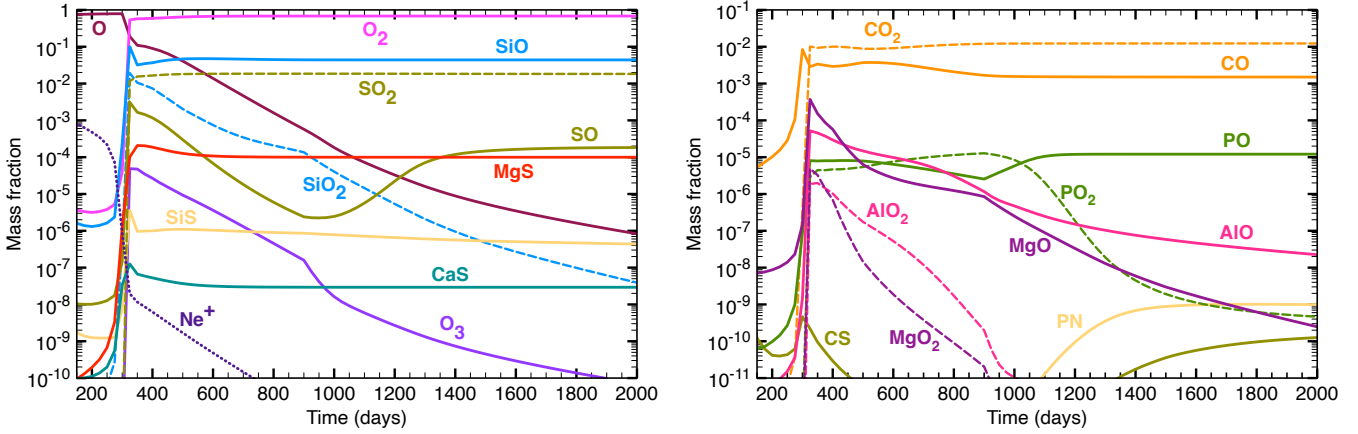
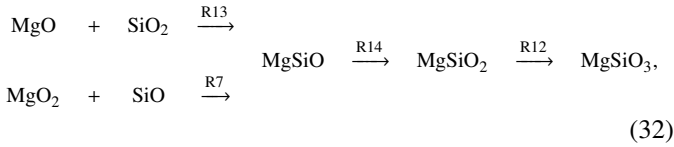
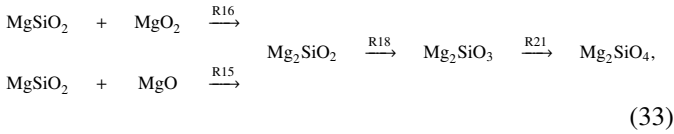


Fig. 6. Mass fractions of main molecules produced in the O/Si/Mg region at $z = 2.15 M_{\odot}$ for the standard case. The zone mass is $5.42 \times 10^{-3} M_{\odot}$.

the ejecta gas reaches the molecular regime with O_2 formation. The enstatite monomer $MgSiO_3$ mainly forms from the reaction sequence,



while for the Mg_2SiO_4 monomer, the reaction sequence is as follows,



where the reaction labels correspond to processes listed in Table 4. At the high gas temperatures around day 300, the moderate endothermicities of reactions R7, R12, and R16 are easily overcome. Finally, the dimers of enstatite and forsterite are formed from reactions R22 and R23 at collisional rate. The $MgSiO_3$ dimers are by far the most abundant in the zone by at least two orders of magnitude compared to Mg_2SiO_4 dimers. Sequences 32 and 33 involve simple and abundant molecules that induce the efficient formation of $MgSiO$ and growth of larger intermediate clusters on short time scales of a few dozen days.

We see from Fig. 7 that in terms of mass fraction, clusters of silica come next, with high mass fraction of Si_3O_5 , followed by Si_3O_6 (the trimer of the SiO_2 unit), and Si_3O_4 . For these three species, the energetically favorable structures are rhombic chains, with adjacent rhombuses perpendicular to each other (Chu et al. 2001; Lu et al. 2003). While Si_3O_5 has one peripheral oxygen atom attached to one rhombus, Si_3O_6 has one peripheral oxygen on each rhombus, implying these two molecules are reactive species that foster chain growth. As mentioned in Sect. 3.2, the sequence for quartz cluster formation starts with the reaction of two SiO_2 molecules to give Si_2O_3 clusters. Subsequent additions of SiO_2 , starting with Si_2O_3 , lead to Si_3O_5 and Si_3O_6 , while reaction of the latter with atomic O leads back to Si_3O_5 . All these processes are exothermic and proceed quickly ensuring these rhombic chains can easily grow by SiO and SiO_2 addition.

Finally, the least abundant dust clusters are of alumina, as seen from Fig. 7. The most abundant species is the linear

Al_2O molecule followed by the kite-shaped cluster Al_3O_3 , and the Al_2O_3 dimer. The formation sequence starts with two AlO molecules reacting together to give Al_2O , which reacts with O_2 to form Al_2O_2 , of rhombus structure (Armstrong et al. 2019). The latter further reacts with O_2 to give the kite-shaped Al_2O_3 cluster. Once formed, Al_2O_3 reacts with O_3 to give Al_2O_4 , which also forms from Al_2O_2 reacting with AlO_3 . Finally, the Al_2O_3 dimer mainly forms out of Al_2O_3 reacting with Al_2O_4 . The most abundant final products Al_2O , Al_3O_3 , and Al_4O_6 have fragmentation energies above ~ 5 eV and are therefore stable, the most stable being Al_4O_6 with its cage structure (Armstrong et al. 2019). However, it appears that for our standard case, the mass fractions of small alumina clusters remain modest compared to other dust clusters.

4.2.2. Total molecule and cluster masses

The total masses of molecules and dust clusters formed over the 145 zones of the O/Si/Mg region are presented in Fig. 8 and values at day 4000 are gathered in Table 5. The formation processes for the various molecules and dust clusters at the zone position $z = 2.15 M_{\odot}$ also operate at other positions in the O/Si/Mg region, albeit with varying efficiencies owing to the different gas conditions and initial elemental compositions.

It emerges that the formation of molecules and dust clusters is not homogenous in the region as seen from Fig. 9, where maps of the masses for SiS, SO_2 , and enstatite dimers are shown as a function of time and zone position in the region. According to Fig. 8, SiS does form with quite high masses in the region. However, we see from Fig. 9 that its formation locus is restricted to zones spanning from the region inner boundary to $\sim 1.92 M_{\odot}$, where the mass fractions of atomic Si and S are still high. The formation of SiS there is residual of the large production of SiS in the Si/S/Ca region, and the molecule cannot be considered as typical of the O/Si/Mg region. By contrast, the formation of SO_2 and $(MgSiO_3)_2$ extends quite homogeneously over the entire region although favoured zones exist for optimal synthesis. For SO_2 , the maximum formation occurs between $1.92 M_{\odot}$ and $1.96 M_{\odot}$ where atomic S and O are abundant before the gradual decrease of atomic sulphur. The formation efficiency gradually drops over the entire region for $z > 1.96 M_{\odot}$. For enstatite dimers, formation is precluded in the very inner zones where SiS is at maximum, while it is favoured from $z = 1.96 M_{\odot}$ and $z = 2.2 M_{\odot}$. The maximum formation efficiency lies between $2.1 M_{\odot}$ and $2.2 M_{\odot}$, where both atomic O, Si and Mg are simultaneously

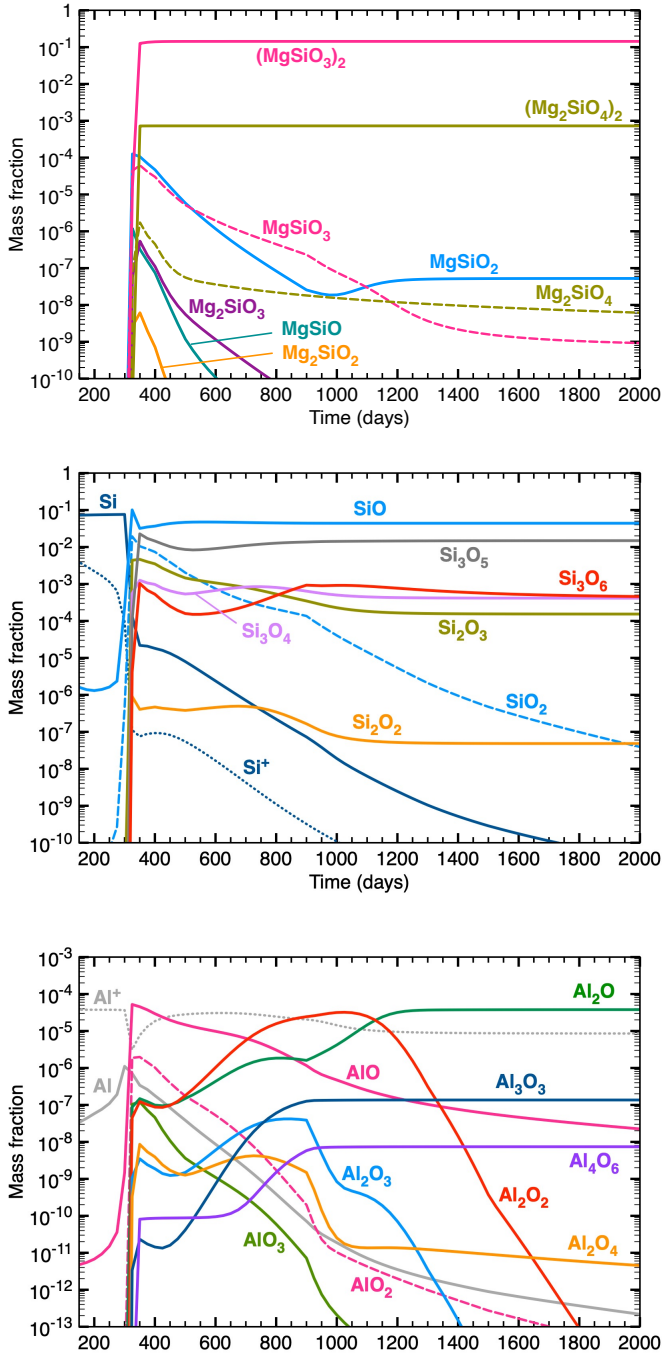


Fig. 7. Mass fractions of dust clusters formed in the O/Si/Mg region at $z = 2.15 M_{\odot}$ versus post-explosion time for the standard case (zone mass = $5.42 \times 10^{-3} M_{\odot}$). Top: Silicates. Middle: Silica (quartz). Bottom: Alumina.

abundant, and drops after $z = 2.2 M_{\odot}$ to stay constant for the rest of the region.

From Table 5, we see the O/Si/Mg region is extremely efficient at forming molecules and dust clusters. The prominent molecules are O_2 , SiO, SO_2 , and CO_2 , and the total molecular mass is $0.525 M_{\odot}$, which represents $\sim 72\%$ of the region's mass. As for dust clusters, the region forms essentially silicate dimers and silica trimers for a total mass of $0.046 M_{\odot}$, equivalent to $\sim 6.3\%$ of the region's mass.

4.3. The O/C/Mg region (outer oxygen region)

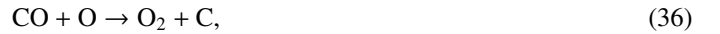
The region is characterised by high O and C initial mass fractions while Mg is still present and the quantity of Si drastically decreases compared to the inner oxygen region. We studied the chemistry in the zone located at $z = 2.7 M_{\odot}$ for which the mass fractions of molecules and silicate clusters are presented in Fig. 10. Because of the large initial content of atomic C, the formation of CO controls the overall chemistry and freezes other molecular synthesis until day 900. Indeed, until day 300, CO is formed out of the fast, temperature-independent charge-exchange reaction,



and destroyed directly by Compton electrons mainly through the process,



The destruction of CO by atomic O,



gradually grows in strength with time to insure the efficient synthesis of O_2 at the expense of CO. At day 700, reaction (36) is the dominant formation process for O_2 while it is destroyed by the formation of SiO following



After day 900, the gas then switches to a molecular formation regime controlled by reactions with O_2 . At that time, dust clusters start forming through the processes discussed in Sect. 4.2. However, we see from Fig. 10 that the mass fraction of silicates is quite low ($\sim 10^{-8}$) at day 4000. Similarly, the mass fraction of silica is $\sim 3 \times 10^{-5}$ when that of alumina clusters is $\sim 1.3 \times 10^{-7}$.

The masses of molecules formed over the entire region are shown in Fig. 11. The prominent species produced in the region are CO, O_2 , and CO_2 . This region synthesises the largest masses of CO and CO_2 in the ejecta as already found in previous studies (e.g. Cherchneff & Dwek 2009), with CO mass growing from day 150 to 400 from $\sim 10^{-4} M_{\odot}$ to over $10^{-1} M_{\odot}$ in good agreement with existing ALMA and recent JWST observations (Kamenetzky et al. 2013; Medler et al. 2025). Interestingly, the region also produces some SiO, SO, and SO_2 with masses at day 4000 of $\sim 2 \times 10^{-4} M_{\odot}$, $4 \times 10^{-5} M_{\odot}$, and $5 \times 10^{-5} M_{\odot}$, respectively.

However, the region contributes modest amounts of dust clusters, the most abundant being silica, followed by alumina and silicates. As in the O/Si/Mg region, no carbon dust clusters form. We find that molecules represent 87% of the region's mass, with a total mass of $0.339 M_{\odot}$, while the dust clusters have a modest mass of $1.46 \times 10^{-5} M_{\odot} \equiv 3.74 \times 10^{-3}\%$ of the region's mass. Although the region has the greatest efficiency at synthesising molecules, it is second to the O/Si/Mg region in terms of molecule masses because the region is of smaller size.

4.4. The He/C/N region (carbon zone)

The He/C/N region expands from $3.013 M_{\odot}$ to $4.141 M_{\odot}$ and is unique for four reasons. Firstly, it has a C/O ratio greater than 10 until $z \sim 3.8 M_{\odot}$. Secondly, the most abundant species is atomic He over the entire region. Thirdly, the region is characterised by a high nitrogen initial mass fraction, N being even more abundant than O and C from $z \sim 3.8 M_{\odot}$ outwards. Finally, fluorine, F, is present at position $z \sim 3.05\text{--}3.6 M_{\odot}$. The only possibility

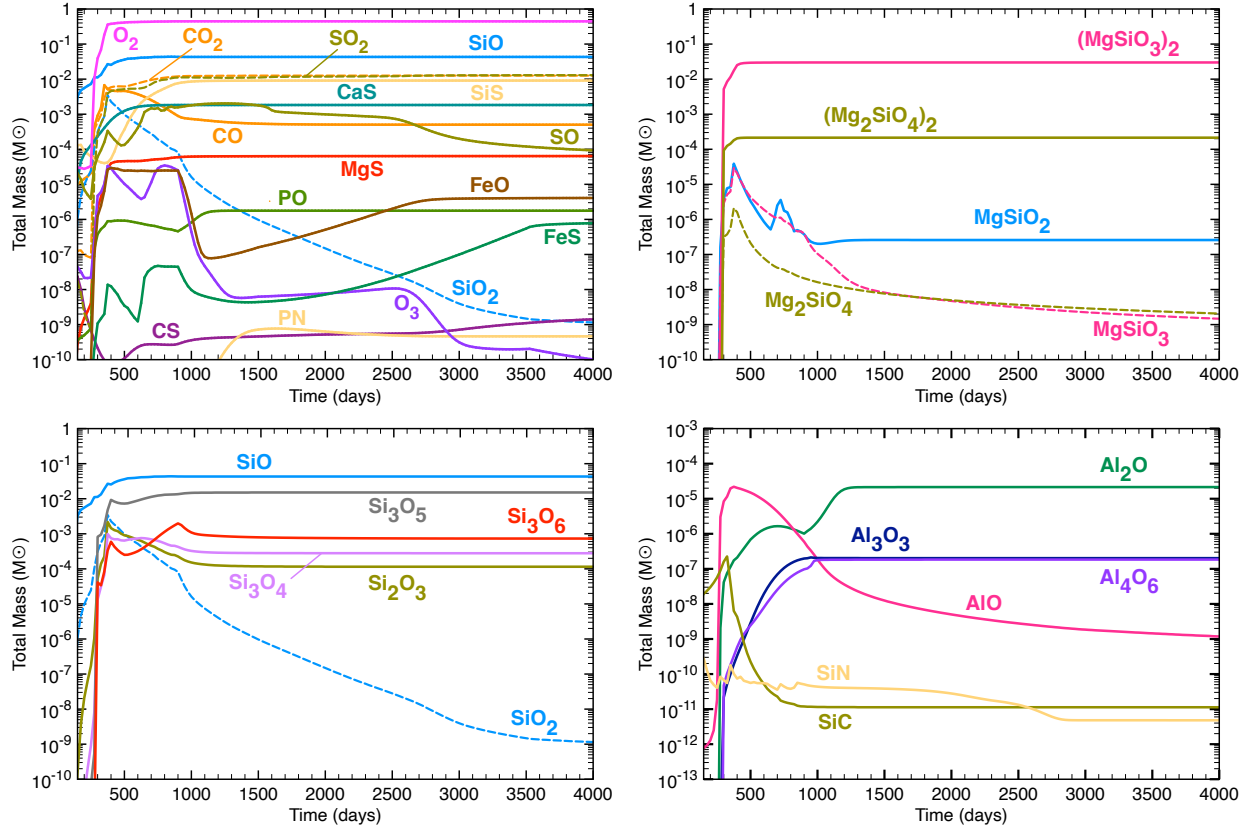


Fig. 8. Total mass of molecules and dust clusters produced in the O/Si/Mg region as a function of post-explosion time for the standard case. Top-left: Molecules. Top-right: Silicates. Bottom-left: Silica. Bottom-right: Alumina. The region mass is $0.729 M_{\odot}$.

for a SN ejecta to form carbon dust resides in this region, since no carbon dust clusters form in the Si/S/Ca, the O/Mg/Si, and the O/C/Mg regions, as we saw previously.

We investigate the chemistry at position $z = 3.3 M_{\odot}$ where $C/O \sim 16$ to highlight the processes conducive to carbon cluster formation. We then study the inner region depleted in N at $z = 3.03$. Finally, we derive the masses of molecules and dust clusters over the entire region.

4.4.1. Molecules and dust clusters at $z = 3.3 M_{\odot}$

Results for molecules and carbon dust clusters are shown in Fig. 12 and reflect the non-straightforward chemistry of the zone. Inspection of Fig. 12 reveals three chemical regimes: the He^+ -controlled regime until day 1400, the C/N/O chemistry regime from day 1300 to 2300, and finally, the regime dominated by carbon chain formation once CO has fully formed.

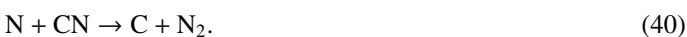
Until day 1300, the formation of molecules (e.g. CO, N_2) is hampered because of the strong destruction by He^+ . Afterwards, CO and N_2 formation becomes efficient but the synthesis of the CN and NO radicals is then responsible for their destruction through the reaction,



while reformation of CO occurs via the following reactions,



along with reaction of atomic C with O_2 . The prominent formation process for N_2 is



When CO synthesis is completed around day 2300, the excess in atomic carbon contributes to the rapid formation of C_2 through the radiative association of two atomic C, while C_3 forms through the reaction,



The carbon chain cycle is then activated whereby small chains grow through radiative association reactions and processes similar to reaction (41), as described by Loison et al. (2014). The abrupt formation of carbon chains around day 2300 is thus due to the completion of the CO synthesis and is unrelated to changes in the gas temperature, which ranges between 110–150 K from day 2200 until day 2400.

The synthesis and growth of larger rings from C_{11} to C_{20} is hindered by the low gas temperatures at day 2300 ($T_{\text{gas}} \sim 125$ K) and no carbon rings larger than C_{10} form in significant amount, as seen in Fig. 12. As explained in Sect. 3.4, the growth of rings larger than C_{10} involves the insertion of C and C_2 units, implying ring opening. These processes have high energy barriers and can only proceed at high enough gas temperatures. Furthermore, the ejecta gas number density after day 2300 is low ($n_{\text{gas}} \leq 1.5 \times 10^6 \text{ cm}^{-3}$, which is at least three orders of magnitude less than n_{gas} at day 100). A low temperature combined to a low number density renders the growth of large carbon clusters unlikely, and a fortiori, the synthesis of carbon dust for the standard case of this study. Most of atomic carbon recycles into C_3 molecules as an end-product, which has a high mass fraction at day 4000. A high number density case for the carbon zone is studied and discussed in Sect. 4.5.

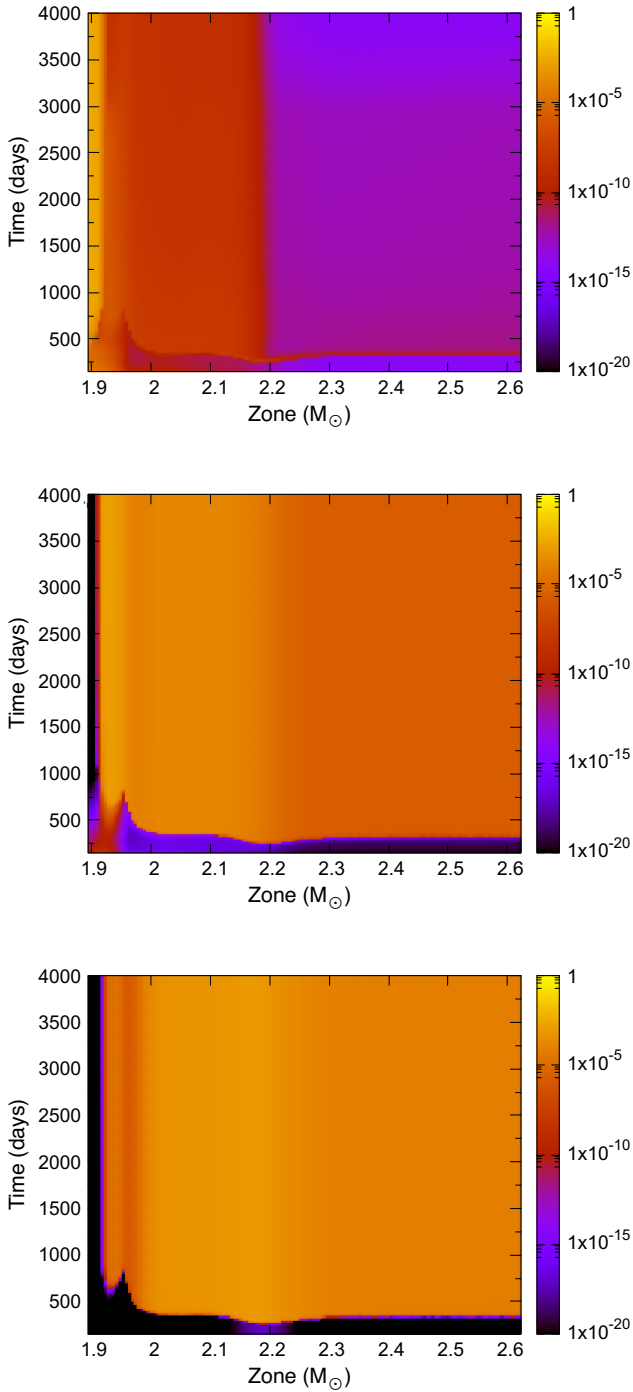


Fig. 9. Mass maps of molecules and enstatite dimers produced in the O/Si/Mg region as a function of time and position z in the region for the standard case: From Top to Bottom: SiS, SO₂, and (MgSiO₃)₂.

4.4.2. Molecules and dust clusters at $z = 3.03 M_{\odot}$

We see from Fig. 1 that there is a zone range $z = 3.013\text{--}3.04 M_{\odot}$, for which atomic C and O have high mass fractions while atomic He mass fraction has not yet reached full value and atomic N mass fraction is low. This small z range corresponds to three zones in total and experiences a different chemistry owing to the peculiar chemical composition.

We show in Fig. 13, the mass fractions for the main molecules and carbon clusters. Results are drastically different from those at $z = 3.3 M_{\odot}$ in terms of timing for molecule and

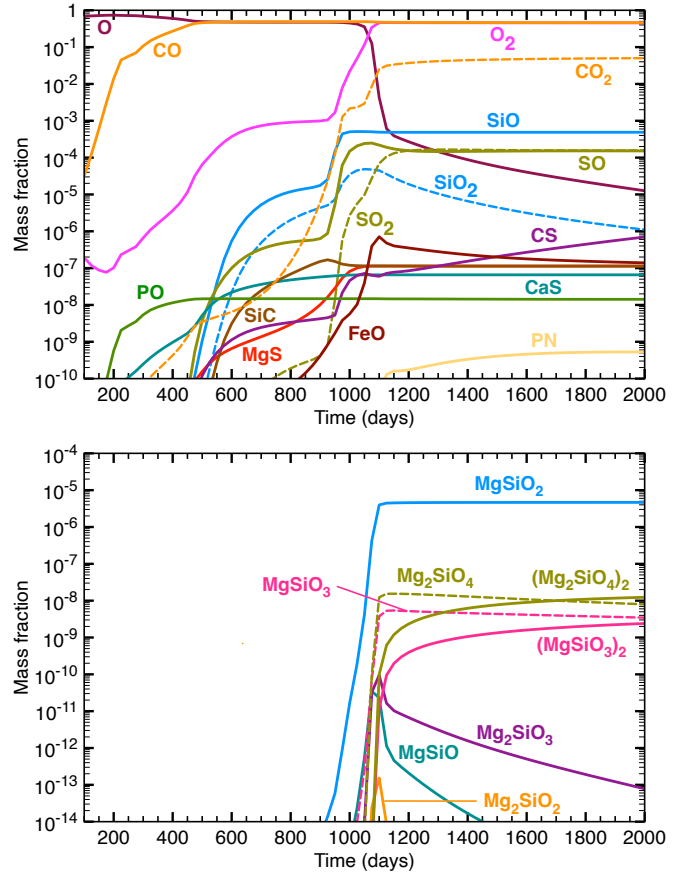


Fig. 10. Mass fractions of molecules and dust clusters formed in the O/C/Mg region at $z = 2.7 M_{\odot}$ versus post-explosion time for the standard case (zone mass = $5.42 \times 10^{-3} M_{\odot}$). Top: Molecules. Bottom: Silicates.

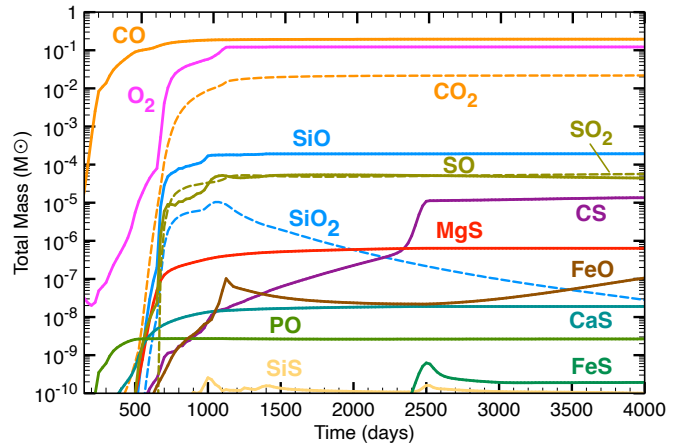


Fig. 11. Total mass of molecules produced in the O/C/Mg region as a function of post-explosion time for the standard case. The region mass is $0.39 M_{\odot}$.

dust cluster production. The combination of a reduced amount of He⁺ and a small N initial content, which shuts down the C/N/O chemistry regime discussed in Sect. 4.4.1, leads to molecule formation around day 1050, where $T_{\text{gas}} \sim 1600$ K and $n_{\text{gas}} \sim 1.5 \times 10^7 \text{ cm}^{-3}$. In contrast with position $z = 3.3 M_{\odot}$, the high gas temperatures allow carbon rings larger than C₁₀ to open and grow, resulting in the formation of C₂₀ with a mass fraction of

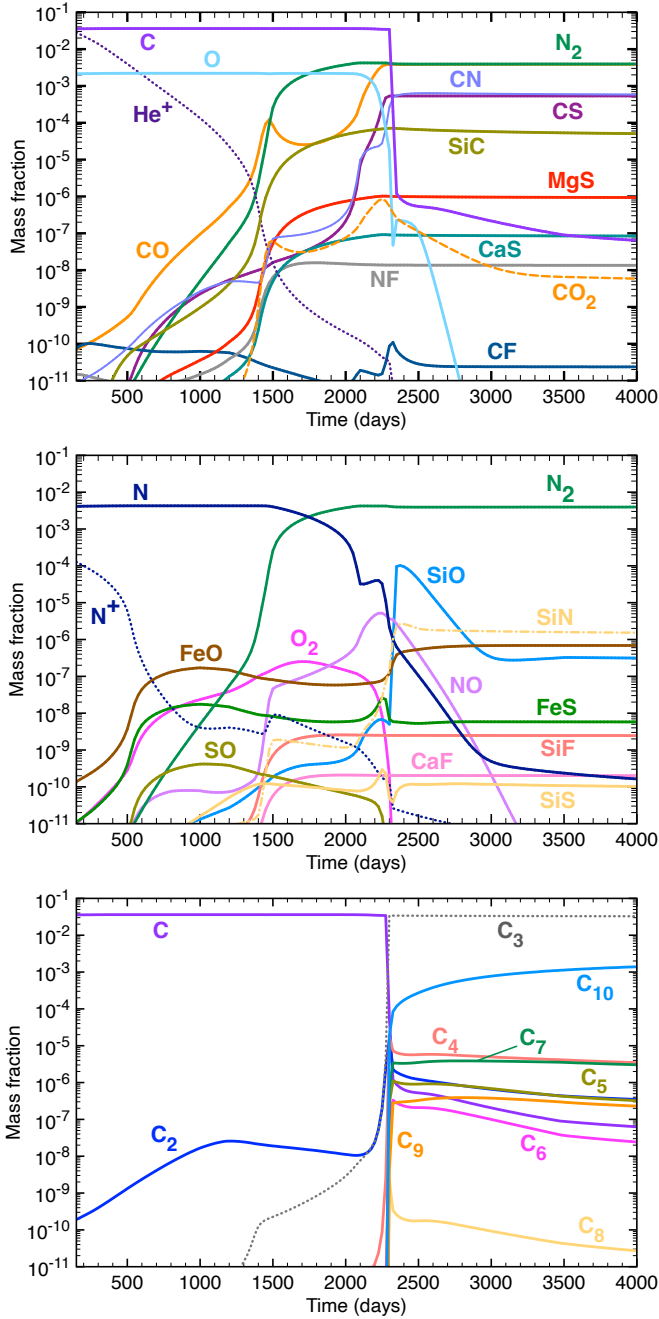


Fig. 12. Mass fractions of molecules and dust clusters formed in the He/C/N region at $z = 3.3 M_{\odot}$ versus post-explosion time for the standard case (zone mass = $1.35 \times 10^{-2} M_{\odot}$). Top and Middle: Molecules. Bottom: Small carbon clusters.

$\sim 4.0 \times 10^{-2}$. For our standard case, the formation of carbon rings over the He/C/N region is reduced to these small inner zones, as we see below.

4.4.3. Total mass of molecules and dust for the He/C/N region

The total masses of molecules formed in the He/C/N region as a function of post-explosion time are presented in Fig. 14. The prominent species are CO, N_2 , and SiO and molecular formation does not proceed before day ~ 800 . The contributions of the three inner zones around $z = 3.03 M_{\odot}$ to the CO mass are clear, and

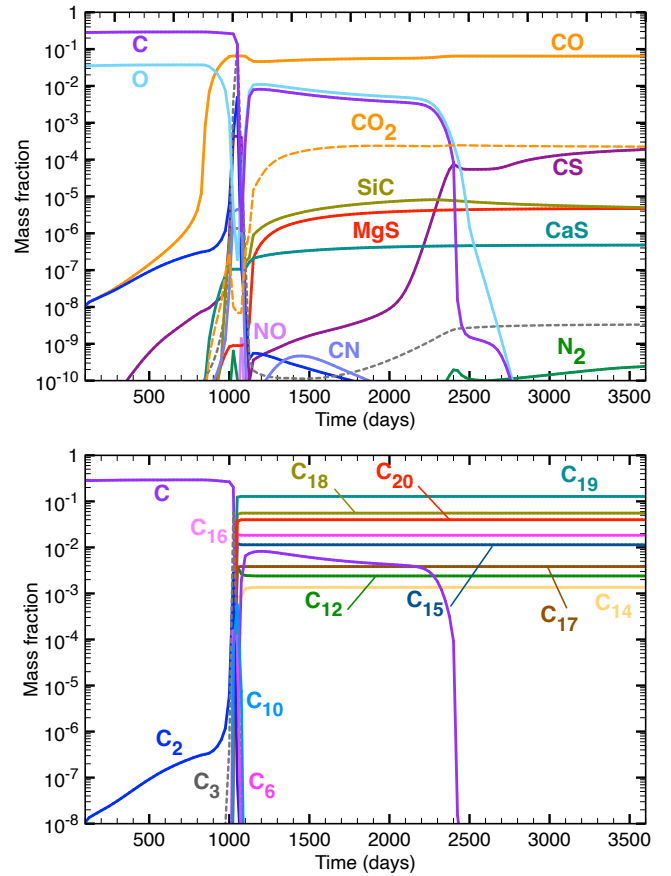


Fig. 13. Mass fractions of molecules and dust clusters formed in the He/C/N region at $z = 3.03 M_{\odot}$ versus post-explosion time for the standard case (zone mass = $1.35 \times 10^{-2} M_{\odot}$). Top: Molecules. Bottom: Carbon clusters.

the CO mass starts rising at day 800. A new increase appears in the CO mass around day 2200 due to contribution to the other zones (e.g. at $z = 3.3 M_{\odot}$ and Fig. 12). N_2 forms in large amount but not before day 1500, while SiO synthesis is delayed to day 2300 in the low-temperature ejecta. We notice the only relevant fluorine-bearing species in the region is NF, which forms along with N_2 and reaches a total mass of $1 \times 10^{-8} M_{\odot}$ at day 4000.

Results for small carbon clusters also reflect the contribution from the three inner zones. The mass of produced C_{20} originates solely from these zones whereas the C_3 mass is primarily produced by the rest of the region until $z \sim 3.8 M_{\odot}$ after day 2300, as seen from Fig. 15, where mass maps for C_3 and C_{20} are displayed as a function of time and position z in the region.

Despite the fact the final C_{20} mass reaches the reasonable value of $\sim 1.5 \times 10^{-3} M_{\odot}$ at day 4000 for our standard case, the formation of the largest carbon clusters is inefficient and restricted to the three inner zones present in the $15 M_{\odot}$ model. However, we notice similar inner zones do exist in the He/C/N region of the $19 M_{\odot}$ progenitor (Rauscher et al. 2002). To circumvent this peculiarity and identify the conditions conducive to efficient carbon dust production, we present below results for a case with high gas density in the He/C/N region.

4.5. High-density case in the He/C/N region

We investigate a high-density (HD) case where the He/C/N region has an initial gas density at day 100 ten times that of the standard case (i.e., $\rho_{HD}(100) = 10 \times \rho_{SC}(100) =$

Table 5. Final masses of molecules and dust clusters (in M_{\odot}) at day 4000 for the full ejecta (standard case).

Species/region	Si/S/Ca	O/Si/Mg	O/C/Mg	He/C/N	Total ejecta	% Ejecta mass
Detected molecules ^a						
CO	2.05×10^{-7}	5.03×10^{-4}	1.95×10^{-1}	5.86×10^{-3}	2.01×10^{-1}	8.52
SiS	4.08×10^{-2}	9.10×10^{-3}	1.00×10^{-10}	4.13×10^{-6}	4.98×10^{-2}	2.11
SiO	9.04×10^{-6}	4.30×10^{-2}	1.92×10^{-4}	6.04×10^{-5}	4.32×10^{-2}	1.83
SO ₂	–	1.30×10^{-2}	5.67×10^{-5}	–	1.31×10^{-2}	0.56
CS	2.54×10^{-7}	1.41×10^{-9}	1.36×10^{-5}	5.02×10^{-4}	5.15×10^{-4}	0.02
SO	–	9.31×10^{-5}	4.43×10^{-5}	4.80×10^{-6}	1.42×10^{-4}	6.02×10^{-3}
Potentially detectable molecules ^a						
O ₂	–	4.45×10^{-1}	1.22×10^{-1}	8.74×10^{-6}	5.67×10^{-1}	24.05
CO ₂	7.57×10^{-9}	1.26×10^{-2}	2.18×10^{-2}	2.13×10^{-5}	3.44×10^{-2}	1.46
C ₃	–	–	–	2.45×10^{-2}	2.45×10^{-2}	1.04
CaS	3.26×10^{-3}	1.83×10^{-3}	1.89×10^{-8}	8.65×10^{-8}	5.09×10^{-3}	0.22
N ₂	–	–	–	2.77×10^{-3}	2.77×10^{-3}	0.12
MgS	1.08×10^{-5}	6.40×10^{-5}	6.37×10^{-7}	9.25×10^{-7}	7.73×10^{-5}	3.28×10^{-3}
CN	–	–	–	4.23×10^{-4}	4.23×10^{-4}	1.79×10^{-2}
Al ₂ O	–	2.15×10^{-5}	1.10×10^{-6}	–	2.26×10^{-5}	9.58×10^{-4}
PO	1.03×10^{-7}	1.77×10^{-6}	2.67×10^{-9}	–	1.88×10^{-6}	7.97×10^{-5}
FeS	3.56×10^{-5}	7.79×10^{-7}	1.92×10^{-10}	3.11×10^{-6}	3.95×10^{-5}	1.68×10^{-3}
FeO	1.55×10^{-10}	4.08×10^{-6}	1.06×10^{-7}	6.48×10^{-7}	4.84×10^{-6}	2.06×10^{-4}
SiO ₂	–	1.15×10^{-9}	2.80×10^{-8}	9.41×10^{-9}	3.86×10^{-8}	1.64×10^{-6}
NF	–	–	–	9.92×10^{-9}	9.92×10^{-9}	4.21×10^{-7}
NO	–	–	–	1.05×10^{-10}	1.05×10^{-10}	4.45×10^{-9}
Total mass	4.41×10^{-2}	5.25×10^{-1}	3.39×10^{-1}	3.42×10^{-2}	9.43×10^{-1}	39.95
Dust clusters ^a						
Mg ₂ Si ₂ O ₆ – enstatite	–	2.99×10^{-2}	9.07×10^{-10}	–	2.99×10^{-2}	1.27
Mg ₄ Si ₂ O ₈ – forsterite	–	2.01×10^{-4}	3.00×10^{-9}	–	2.10×10^{-4}	8.91×10^{-3}
Si ₃ O ₅ – quartz	–	1.51×10^{-2}	1.02×10^{-5}	–	1.51×10^{-2}	0.64
Si ₃ O ₆ – quartz	–	7.31×10^{-4}	8.29×10^{-7}	–	7.32×10^{-4}	3.10×10^{-2}
Al ₄ O ₆ – alumina	–	1.84×10^{-7}	1.90×10^{-10}	–	1.84×10^{-7}	7.81×10^{-6}
C ₂₀ – carbon	–	–	–	1.53×10^{-3}	1.53×10^{-3}	6.49×10^{-2}
SiC – silicon carbide	–	–	3.54×10^{-6}	3.56×10^{-5}	3.91×10^{-5}	1.66×10^{-3}
SiN – silicon nitride	–	–	–	1.38×10^{-6}	1.38×10^{-6}	5.85×10^{-5}
Total mass	–	4.59×10^{-2}	1.46×10^{-5}	1.57×10^{-3}	4.75×10^{-2}	2.02

Notes. ^(a) Masses less than $10^{-10} M_{\odot}$ are labelled as –.

$1.35132 \times 10^{-12} \text{ g cm}^{-3}$). A factor of 10 is a reasonable choice of over-density factor assuming clumping in the ejecta with a volume filling factor, $f_v = 0.1$. We recall the density in the clump, ρ_g , verifies the equation,

$$\rho_g \times f_v = \rho_c, \quad (42)$$

where ρ_c is the core gas density given by Equation 11 (Truelove & McKee 1999). The HD case corresponds to a number density at day 100 of $n_{\text{gas}}(100) \sim 2 \times 10^{11} \text{ cm}^{-3}$ for the ejecta gas in the He/C/N region. Such a value is comparable to values derived at day 100 for the clumpy ejecta of SN1987A and SN2005af (Sarangi 2022; Sarangi et al. 2025). However, the present $n_{\text{gas}}(100)$ value is about two orders of magnitude smaller than the number density for the clumpy case of Sarangi & Cherchneff (2015).

Results for carbon clusters at $z = 3.3 M_{\odot}$ are presented in Fig. 16 (Top) and have to be compared with results for the standard case of Fig. 12. The higher gas densities allow a faster recombination of He⁺ so that molecules start forming at day 1000, and squeeze the C/N/O chemistry regime discussed in Sect. 4.4.1 to the time range day 1000–1250. After day

1250, characterised by $T_g \sim 1000 \text{ K}$ and $n_g \sim 1 \times 10^9 \text{ cm}^{-3}$, carbon clusters form quickly and grow efficiently to carbon rings, including C₂₀, because ring opening and growth through C and C₂ inclusion is made possible at these gas temperatures.

The total masses of molecules and carbon clusters are also shown in Fig. 16 (Middle and Bottom, respectively), while we gather all molecule and cluster masses for the HD case as a function of region and at day 4000 in Table A.3 of the Appendix. The masses of most molecules have increased because the formation of species now occurs earlier and at higher densities. The increase is particularly strong for N₂ and CN, whose mass at day 4000 is about ten times higher than for the standard case. As for carbon clusters and large rings in particular, we now see two contributions: one by the three inner zones at day 700–800 and a strong contribution at day 1200–1300, which double the mass of C₂₀. This double contribution is amply supported by the data in Fig. 17, where mass maps of both C₃ and C₂₀ for the high-density case are shown. The mass of C₂₀ is now distributed from the inner edge of the region to $z = 3.8 M_{\odot}$, the starting point of the N-rich sub-region. In the end, the density enhancement has increased the total mass of C₂₀ at day 4000 by a factor

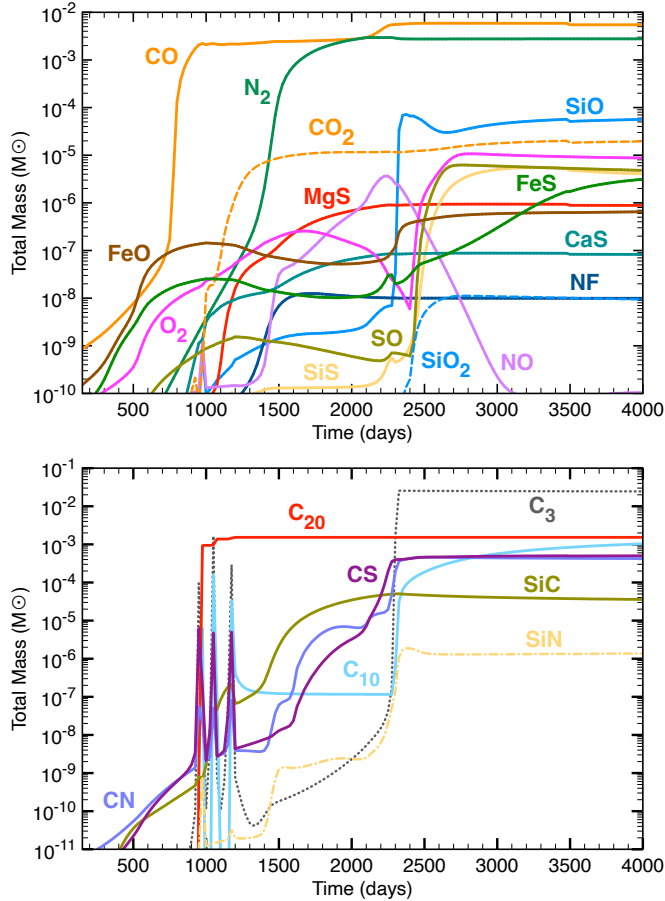


Fig. 14. Total mass of molecules produced in the He/C/N region versus post-explosion time for the standard case Top: Molecules. Bottom: Carbon clusters, C-bearing radicals, SiC, and SiN. The region mass is $1.128 M_{\odot}$.

five. Interestingly, small carbon chains and rings do form after day 2300, but do not grow larger than C_{10} , as a result of the low-temperature chemistry characterising the formation of small carbon chains (Loison et al. 2014).

We conclude the synthesis of carbon dust is greatly favoured in dense clumps as opposed to other types of dust like silicates or silica, which form efficiently for the gas conditions of the standard case. The existence of the narrow carbon-cluster-forming region at the inner edge of the He/C/N region is present in both explosion models for 15 and $19 M_{\odot}$ progenitors by Rauscher et al. (2002). Therefore, we expect a similar early carbon cluster synthesis from a few inner zones in the ejecta of a $19 M_{\odot}$ progenitor. However, this specific region may not be present in the initial elemental composition of SN explosion models with progenitors that are more or less massive than this level. This situation does not invalidate our finding that carbon clusters require dense gas to form in significant amount in the ejecta. Furthermore, we expect the small chain C_3 to always be present in the gas at day 4000. Indeed, despite the fact the molecule participates in the formation of carbon clusters at earlier times, there is a residual C_3 population at day 4000 as a result of the low-temperature chemistry responsible for small carbon chain production. The lower the gas density, the larger the C_3 population, and, thus, the molecule can be seen as a tracer of diffuse carbon-rich ejecta gas.

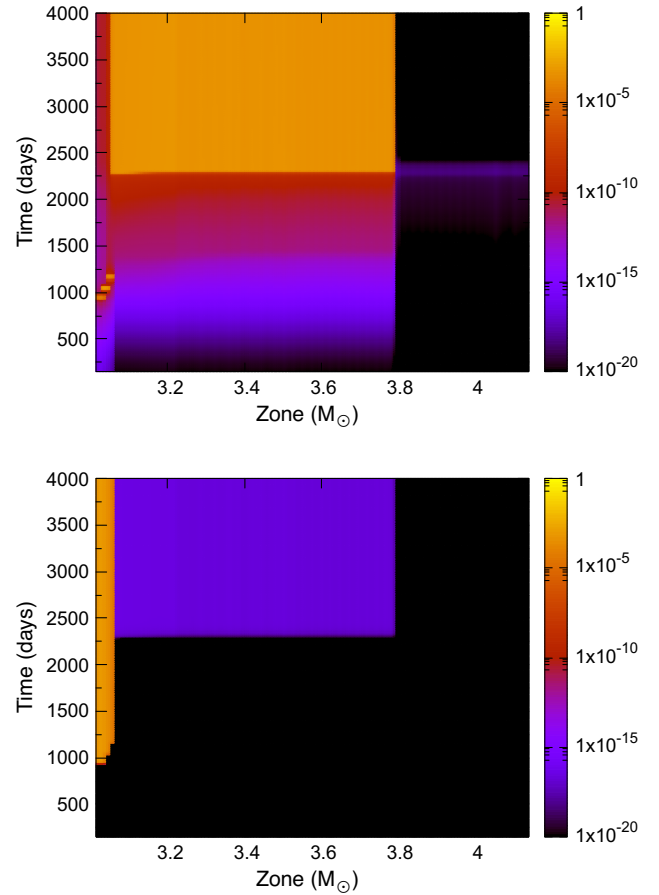


Fig. 15. Mass maps of small carbon clusters produced in the He/C/N region as a function of time and position, z , in the region for the standard case. Top: C_3 . Bottom: C_{20} .

4.6. Low-temperature case in the O/Si/Mg region

In their study of the temperature of the oxygen core in SN 1987A, Liu & Dalgarno (1995) were the first to assess cooling by vibrational emission lines of CO in the O/C/Mg region. This cooling is again investigated in SN 1987A through an exhaustive radiative transfer study by Liljegren et al. (2020), who show the gas temperature drops by at least 1000 K compared to cases without molecular cooling, as for example in Kozma & Fransson (1998). We recall we use in this study the temperature profile derived by Liljegren et al. (2020) for the O/C/Mg region of the ejecta. Cooling might occur in the O/Si/Mg zone as well, specifically through vibrational emission of SiO, which is very abundant in this region, as first mentioned by Liu & Dalgarno (1995) who expected the impact on the gas temperature to be close to that of CO in the O/C/Mg region.

We therefore considered the case of low gas temperature (LT case) in the silicate-forming region by applying the temperature profile of the O/C/Mg region as derived by Liljegren et al. (2020) to the O/Si/Mg region. In the Appendix, the results are presented in Fig. A.1 and molecule and cluster masses at day 4000 are listed in Table A.3. When molecular masses are slightly enhanced, we see the most important changes involve dust clusters: the mass of produced silicates is smaller than that for the standard case (see Fig. 8) by a factor ~ 300 , while the mass of silica clusters slightly increases by $\sim 6\%$, and that of alumina drastically drops by \sim five orders of magnitude. The total cluster mass budget is about three times lower than for the

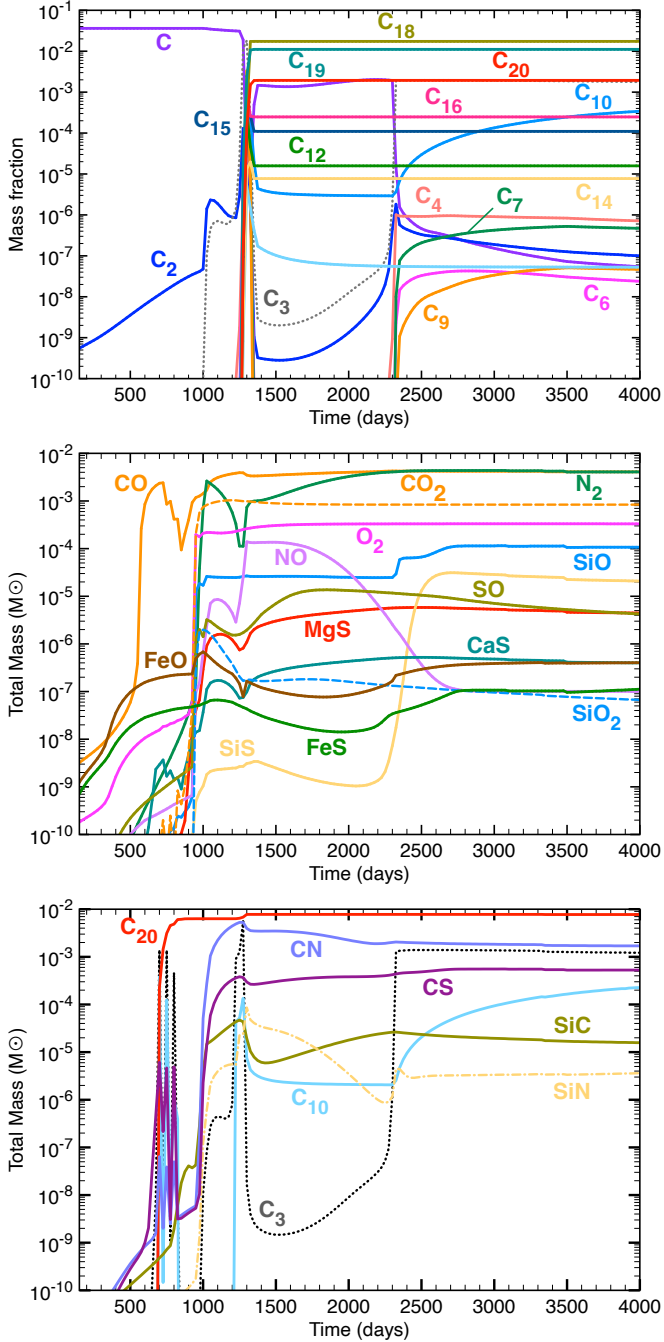


Fig. 16. Top: Mass fractions of carbon clusters formed in the He/C/N region at $z = 3.3 M_{\odot}$ versus post-explosion time for the high-density case (zone mass = $1.35 \times 10^{-2} M_{\odot}$). Middle: Total masses of molecules formed in the He/C/N region as a function of post-explosion time for the high-density case. Bottom: Total masses of carbon clusters formed in the He/C/N region as a function of post-explosion time for the high-density case.

standard case. The main reason to the strong decrease in silicate production is due to reaction R12 of our proposed new scheme for silicate formation (see Table 4). R12 is endothermic with a moderate barrier of ~ 5000 K and the main channel to the formation of MgSiO_3 monomers. The lower gas temperatures between day 200 and 500 thus reduce the efficiency of the process. Since Mg_2SiO_4 monomers form out of MgSiO_3 units, masses of both silicate dimers are drastically reduced. We deduce that reason-

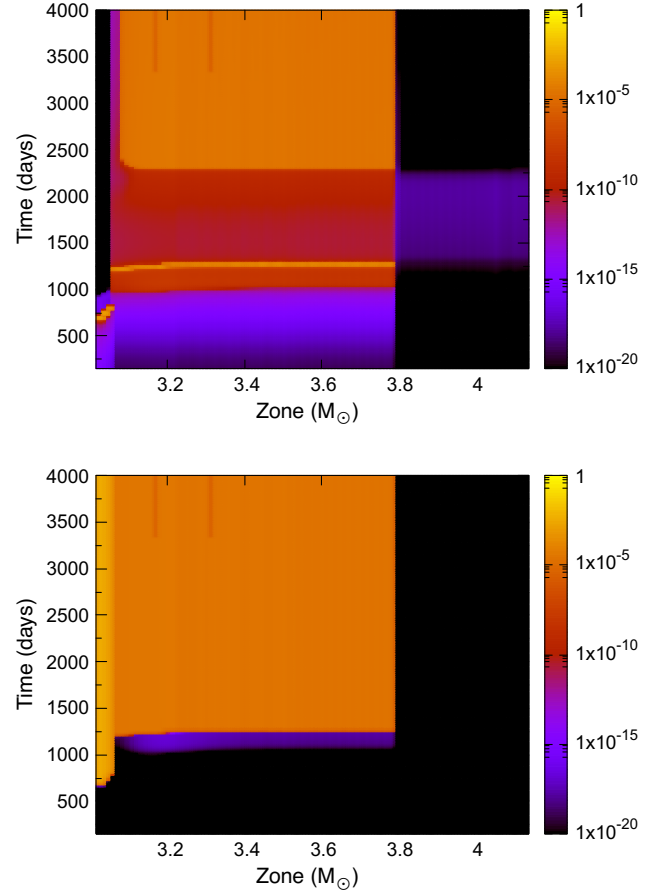


Fig. 17. Mass maps of small carbon clusters produced in the He/C/N region as a function of time and position, z , in the region for the high-density case. Top: C_3 . Bottom: C_{20} .

ably high gas temperatures are required to boost silicate formation according to our new proposed scheme.

From our two tests on gas density and temperature, we find that the inferred high gas densities and temperatures are a prerequisite to efficient dust synthesis in the gas, implying dust must form at early times in the evolution of the ejecta, as shown by previous models (e.g. Cherchneff & Lilly 2008; Cherchneff & Dwek 2010; Sarangi & Cherchneff 2015). Our findings are in conflict with a late dust formation scenario for the remnant of SN1987A, as suggested by Wesson et al. (2015) to fit multi-wavelength astronomical data. They also question the late carbon dust formation scenario at $t > 2400$ days for SN1987A, as proposed by Sarangi (2022) to fit the same near- and mid-infrared data. Our results show no carbon clusters in the form of large rings that act as coagulation seeds, can form at these late times and low gas temperatures. On the other hand, our model allows for the formation of carbon clusters with high masses at day 500 and day 1200 for gas densities and temperatures similar to those used by Sarangi (2022).

5. Comparison with observations

Although this study refers to the 1D, stratified, spherical ejecta of a $15 M_{\odot}$ SN template, drawing a comparison between the present predictions and existing astronomical data is instructive enough and helps identifying the chemistry at play in real SN ejecta, which are usually clumpy and result from various explosion configurations and progenitor masses. Therefore, we discuss and

compare results on molecules and dust clusters with available data on several Type II-P SNe.

5.1. CO

The first overtone bands ($\Delta v = 2$) of carbon monoxide CO located at 2.3–2.5 μm are observed as early as day 112 until day 349 in SN 1987A (Spyromilio et al. 1988), from day 124 till day 205 in SN 2017eaw (Rho et al. 2018), and recently from day 199 till day 307 in SN 2023ixf (Park et al. 2025). Recent JWST data on SN 2023ixf by Medler et al. (2025) show the excitation of both the first overtone bands and the fundamental bands ($\Delta v = 1$) near 4.6 μm at day 252 while at day 373, the first overtone bands already fade owing to gas cooling while the fundamental bands are still excited. An early CO formation is also predicted by chemical models (Lepp et al. 1990; Cherchneff & Lilly 2008; Cherchneff & Dwek 2009; Sarangi & Cherchneff 2013; Sluder et al. 2018).

Our new model confirms an early CO formation around day 200, as seen in Fig. 18, where mass maps of CO for the entire ejecta are presented as a function of time and z position. Firstly, we see that CO is produced in all ejecta regions although with very small efficiency in the Si/S/Ca region. While it forms quite homogeneously as early as day 200 in the two regions of the oxygen core, the O/C/Mg region is by far the most efficient of the two at forming CO, as already found by Liu & Dalgarno (1995) and Cherchneff & Dwek (2009). CO also forms in the outer carbon-rich region, but not before day 750 and with an inhomogeneous distribution and a smaller efficiency in space and time compared to the previous region. An early CO synthesis is also seen in Fig. 20 where the total masses of CO and SiO are shown as a function of time and regions, along with masses derived from the above observations and NIR and ALMA data of SN1987A. Clearly, about $10^{-4} M_{\odot}$ of CO forms at day 200, in accord with observations, and grows to reach $\sim 0.2 M_{\odot}$ at day 3000. This mass at late times agrees well with the CO line analysis of ALMA data by Matsuura et al. (2017).

5.2. SiO

The fundamental band of SiO between 7.5–9 μm was detected and the emission modelled in a few SNe: in SN1987A, from day 260 and 519 (Roche et al. 1991; Liu & Dalgarno 1994), in SN 2005af at day 214 (Kotak et al. 2006), and in SN 2004et, between day 300 and 795 (Kotak et al. 2009). Interestingly for this last object, the SiO emission decrease with post-explosion time was correlated to the onset of dust formation. The modelled SiO masses were comprised between $\sim 10^{-4}$ – $10^{-3} M_{\odot}$. The molecule is also detected in SN 1987A with ALMA at much later times and the line analysis results in a SiO mass ranging between 4×10^{-5} and $2 \times 10^{-3} M_{\odot}$ (Matsuura et al. 2017).

We present mass maps of SiO for the entire ejecta in Fig. 19 as a function of time and z position as well as the total masses of SiO as a function of time and regions in Fig. 20. Inspection of Fig. 19 reveals that SiO forms in all ejecta regions but with rather low masses except for a maximum reached in the silicate/silica-forming region O/Si/Mg, between 1.9 and 2.2 M_{\odot} , where the initial Si mass fraction is large. The SiO distribution also shows more inhomogeneities compared to that of CO and the molecule forms at later times, especially in region O/C/Mg and He/C/N. We see from Fig. 20 that the SiO mass increases with time and shows a reasonable agreement with astronomical data before day 500. It reaches a value of $\sim 4 \times 10^{-2} M_{\odot}$ at day 4000 (see also Table 5), which is larger than the upper limit of

SiO mass derived from ALMA data by more than a factor of ~ 20 . However, we see at least two reasons for not being alarmed by such a difference. Firstly, SN 1987A has a progenitor mass of 19 M_{\odot} with different initial elemental composition and explosion configuration. Secondly, this study only investigates the molecular component of a fictitious, spherically symmetric ejecta and not the solid component, which will form out of cluster coagulation and surface deposition. We believe surface deposition of SiO and SiO-related species onto silicate and silica grains at late time may reduce the final SiO mass.

One positive aspect is that our new chemical model does not totally deplete the SiO mass as the former model did because we use a novel chemical description of the formation of silicate clusters where SiO dimerisation plays a minor role. Indeed, Sarangi & Cherchneff (2013) find the SiO mass drastically decreases from day 200 to 1500, where the mass is $\sim 10^{-6}$ and already much less than the lower SiO mass limit found from ALMA data. A similar low SiO mass is derived in a recent study of SN 2005af by Sarangi et al. (2025), where the same chemical model as of Sarangi & Cherchneff (2013) is used and the SiO mass has already dropped to $\sim 10^{-5} M_{\odot}$ at day 1000. We are thus encouraged by the present findings and will derive final SiO masses when modelling dust synthesis.

Finally, our results cannot explain the 3D SiO distribution in SN 1987A as reconstructed by Abellán et al. (2017) whereby SiO extends to greater radial distances (\equiv higher velocities) than CO in some directions, but where most of the CO emission presents a maximum extension larger than that of SiO. Here, we investigate a 1D physico-chemical model applied to a spherically-symmetric, stratified ejecta and apply a unique chemical model to the entire ejecta regions. However, our findings confirm most of the SiO mass forms inwards to that of CO, in agreement with the reconstruction, and shows SiO formation in the outer ejecta region (i.e. at higher velocities). Furthermore, both CO and SiO distributions are stratified but the latter shows more inhomogeneities resulting from chemistry, specifically in the oxygen core and the outer He/C/N region. Therefore, we propose chemistry may contribute to some extent to the spread and inhomogeneous SiO distribution in SN 1987A, on top of dynamic instabilities, as suggested by Abellán et al. (2017).

5.3. Other molecules

A few other species are identified in the ejecta of SN 1987A, and include SO, SO₂, SiS, and CS.

Sulphur monoxide, SO, is predicted to form in the oxygen core of SNe a few years after the outburst by theoretical models (Cherchneff & Dwek 2009; Sarangi & Cherchneff 2013) and detected with ALMA in SN1987A decades after explosion (Matsuura et al. 2017). The derived mass from line analysis is $4 \times 10^{-5} M_{\odot}$. The present total modelled mass is $1.4 \times 10^{-4} M_{\odot}$ and is consistent with ALMA observations. The molecule is essentially formed in the O/Si/Mg region that produces silicates and silica, and in the O/C/Mg region, which forms most of CO.

We have also predicted the formation of a large quantity of sulphur dioxide, SO₂, in the O/Si/Mg region, with a mass of $1.3 \times 10^{-2} M_{\odot}$. Lines of SO₂ are tentatively identified in the ALMA spectral coverage of SN 1987A. However, the SO₂ lines are weak or blended with other lines (e.g. HCO⁺) and no mass is derived (Matsuura et al. 2017). Therefore, a strong disagreement exists between our large SO₂ mass formed in the first years after the explosion and that derived from ALMA data, unless SO₂ is partially withdrawn from the ejected gas by some chemical or physical processes. In the context of the study of volcano

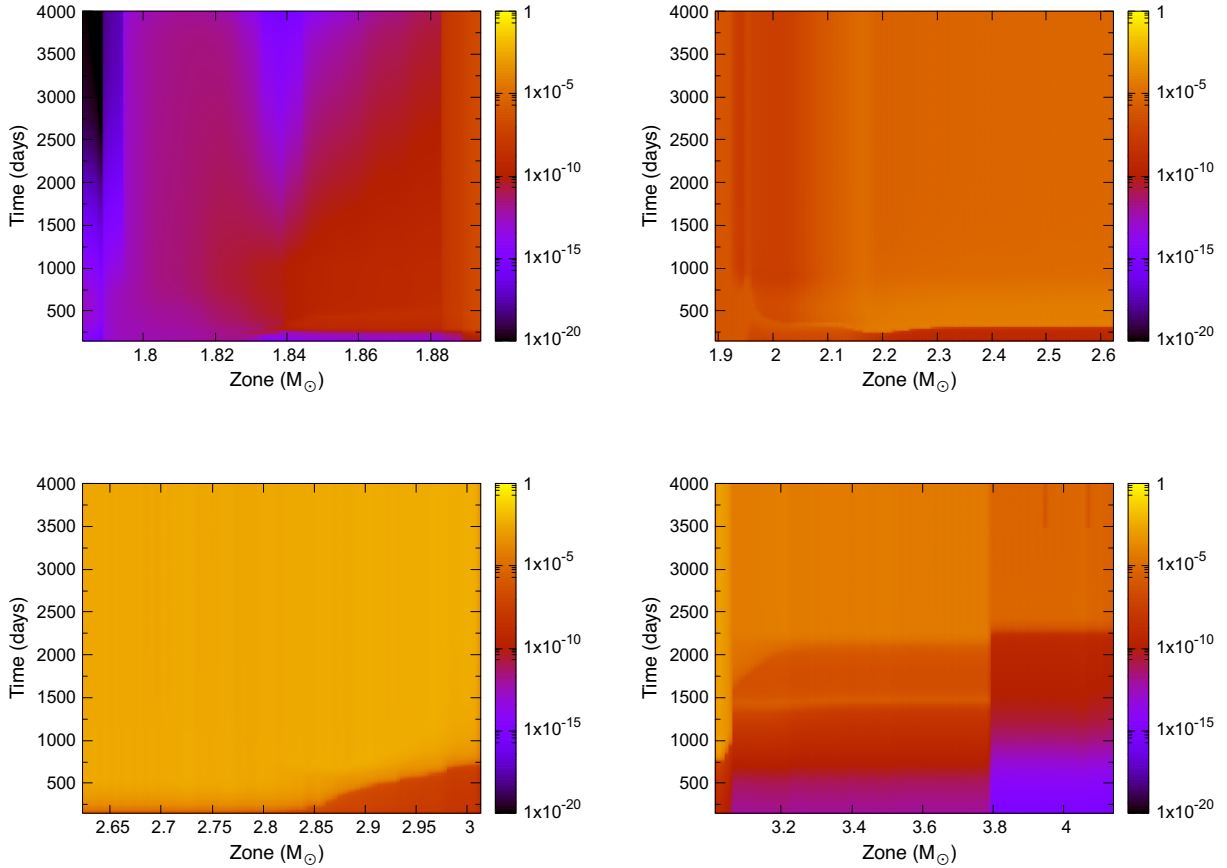


Fig. 18. CO mass maps for the standard case. Top-left: Si/S/Ca region. Top-right: O/Si/Mg region. Bottom-left: O/C/Mg region. Bottom-right: He/C/N region.

gas plume interaction with solid ashes during volcanic eruptions or gas-aerosol interaction on planets and exoplanets, the reaction of hot/warm gaseous SO_2 on the surface of silicate glasses is studied and results in SO_2 depletion and formation of solid sulphates and silica in the case the solid is olivine (King et al. 2018). SO_2 and silica/silicates having the same formation locus in the ejecta, we suggest depletion of SO_2 from the gas phase might occur through a similar process.

As discussed in Sects. 4.1 and 4.2.2, silicon monosulphide, SiS, is the prominent species formed in the Si/S/Ca region, while a residual mass is also produced in the O/Si/Mg region. The total SiS mass at day 4000 is large with a value of $\sim 5 \times 10^{-2} M_\odot$ (see Table 5). The molecule is tentatively identified at late times in SN 1987A with ALMA and a mass upper limit of $6 \times 10^{-5} M_\odot$ is estimated (Matsuura et al. 2017). This is much less than the value we derive a few years after explosion, even when considering differences in initial elemental compositions owing to the different progenitor masses ($15 M_\odot$ for our study and $19 M_\odot$ for SN1987A). However, we do not consider the synthesis of the non-organic solid SiS_2 in our model. Solid silicon disulphide was proposed as a potential carrier of the $21 \mu\text{m}$ band observed in proto-planetary nebular (Goebel 1993). Glassy SiS_2 shows a strong emission band around $\sim 20 \mu\text{m}$ and a minor peak at $16.5 \mu\text{m}$ (Begemann et al. 1996). If SiS_2 clusters were to form in significant amount, we would expect the final mass of SiS to decrease in the inner ejecta regions. The formation of solid SiS_2 will be investigated in a forthcoming paper.

Finally, the first-overtone emission of carbon sulphide, CS, is tentatively identified around $3.88 \mu\text{m}$ in SN 1987A a

few hundred days after outburst (Meikle et al. 1989, 1993) and at late times with ALMA (Matsuura et al. 2017). Existing models (Lepp et al. 1990; Cherchneff & Dwek 2009; Sarangi & Cherchneff 2013) predict a mass between 10^{-5} and $10^{-4} M_\odot$, whereas an upper limit of $7 \times 10^{-6} M_\odot$ is derived from ALMA data. We find CS forms essentially in the He/C/N regions with a mass of $5 \times 10^{-4} M_\odot$ at day 4000. An inspection of Figs. 14 and 16 reveals CS does respond to gas density enhancement by shifting its formation onset from day 1000 for the standard case to day 500 for the high-density case. The final masses in both cases are rather similar. In any case, we see an early detection of CS cannot arise prior to a few hundred days after explosion and it traces the density of the ejecta gas. According to our model, the cyano radical, CN, forms along with CS in the C-rich region, showing a similar trend in the onset of its formation. As such, it can also be regarded as a gas density tracer through the detection of its fundamental band at $5 \mu\text{m}$ in the near IR (Civiš et al. 2023).

Apart from SO, SO_2 , SiS, and CS, a number of molecules form in large amounts in the ejecta but are not yet observed in SN environments. They are O_2 , CO_2 , C_3 , and CaS, and are all detected in space. Sub-millimetre transitions of O_2 between 119 GHz and 1121 GHz were observed in molecular clouds with the Submillimeter Wave Astronomy Satellite (Melnick et al. 2000), the Odin Satellite (Larsson et al. 2007), and the Herschel Space Observatory (Goldsmith et al. 2011). The CO_2 molecule is important as coolant through emission in the v_2 bending mode at $15 \mu\text{m}$ in planetary atmospheres (Kutepov & Feofilov 2024). The antisymmetric stretch v_3 mode of C_3 at $\sim 4.9 \mu\text{m}$ was observed in the carbon-rich AGB star IRC+10216 (Hinkle et al.

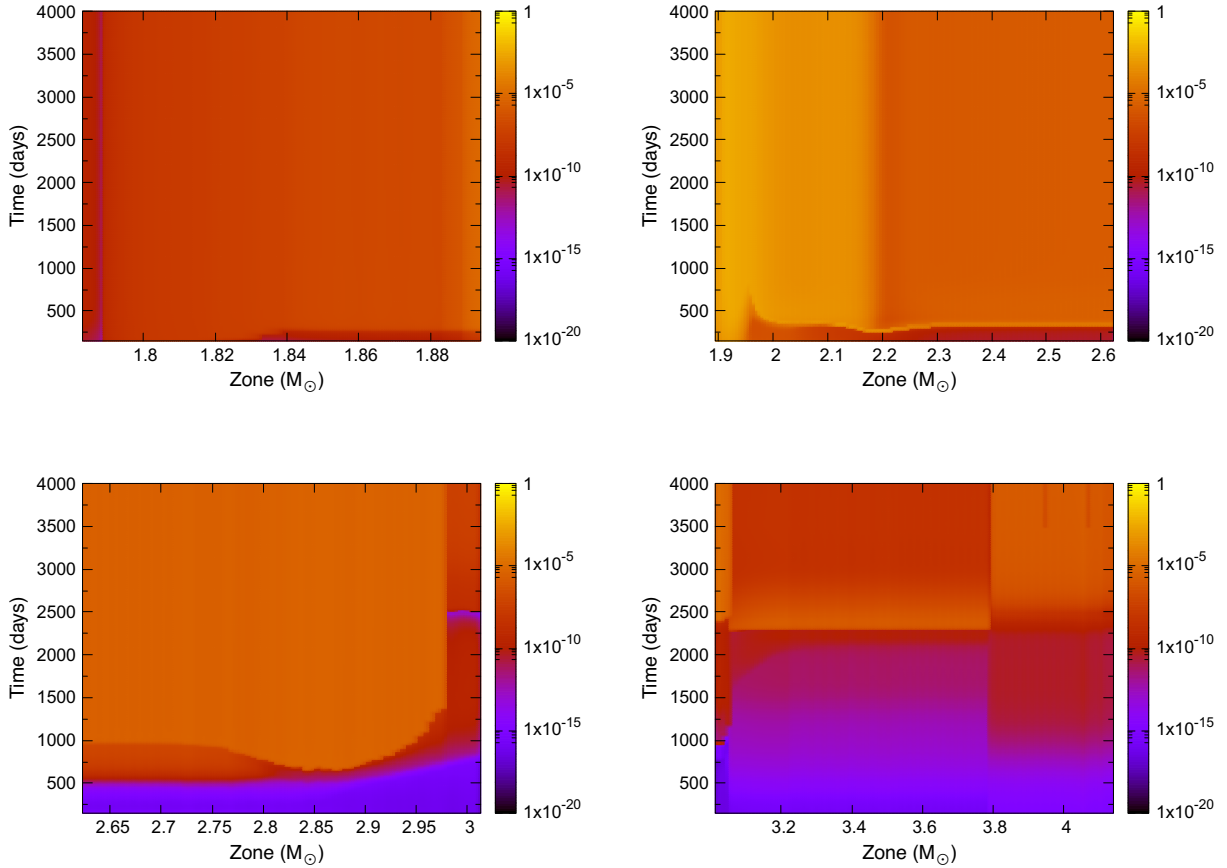


Fig. 19. SiO mass maps for the standard case. Top-left: Si/S/Ca region. Top-right: O/Si/Mg region. Bottom-left: O/C/Mg region. Bottom-right: He/C/N region.

1988) while the presence of the molecule was confirmed in the same object through observation of the ν_2 bending mode at $\sim 150 \mu\text{m}$ with the Infrared Space Telescope (Cernicharo et al. 2000). As for CaS, the rotational lines identified in the laboratory by Takano et al. (1989) were tentatively detected with ALMA in the disc around the massive young stellar object G351.77-0.54-mm1 in the ISM (Tasa-Chaveli et al. 2025).

5.4. Dust clusters

We present in Fig. 21 the masses of dust clusters derived for the standard case, the standard case with a high-density He/C/N region, and the standard case with a low-temperature O/Si/Mg region. We also plot the dust masses derived from observations of a number of Type IIP SNe and SN 1987A. Since we deal only with the ejecta molecular phase in this paper and do not model the coagulation and growth of the dust clusters we consider, the mass values of Fig. 21 provide indications on the final dust mass but does not reflect the time evolution of dust grains, specifically the time at which coagulation of clusters begins to be efficient.

The coagulation efficiency involves two opposite processes, the adhesion mechanisms due to interaction forces and the thermal rebounds effects directly linked to the translational kinetic energy of the particles, and thus the gas temperature. At high temperature, thermal rebounds prevails and coagulation efficiency greatly diminishes (Johannessen et al. 2001; Sirignano & D’Anna 2013). It is therefore reasonable to consider coagulation initiates at the temperature regime of flame

experiments. For the low-temperature case of region O/Si/Mg, the synthesis of silica and silicate clusters starts at \sim day 250 where $T_{\text{gas}} \sim 1600 \text{ K}$, implying the clusters of Fig. 21 will readily coagulate while this may not be the case for the standard case, where silica and silicate clusters start forming around day 300 and at $T_{\text{gas}} \sim 3500 \text{ K}$. In this case, coagulation will start at later times.

Besides coagulation issues, we see the mass derived from observational data shown in Fig. 21 are consistent with modelling trends for cluster formation with a better agreement when lower temperatures are considered for the O/Si/Mg region. Since this region produces large quantities of SiO, it would be of interest to consider SiO cooling when deriving temperature profiles for this zone. These trends agree also with recent observations of SN 2023ixf with the JWST reported by Medler et al. (2025). They find the detection of CO bands at day 252 is accompanied by a dust emission growing in strength relative to the SN flux around $10 \mu\text{m}$ and an excess in flux at $18 \mu\text{m}$, indicative of silicate and silica dust (Jäger et al. 2003).

6. Comparison with other modelling studies

Several studies have partially (Sluder et al. 2018; Liljegren et al. 2020) or entirely (Sarangi 2022; Sarangi & Slavin 2022; Sarangi et al. 2025) used the chemical scheme developed by Cherchneff & Lilly (2008), Cherchneff & Dwek (2009) and Sarangi & Cherchneff (2013). This scheme was a first attempt in the description of the formation of molecules and dust molecular clusters in a H-free environment, drawing on available

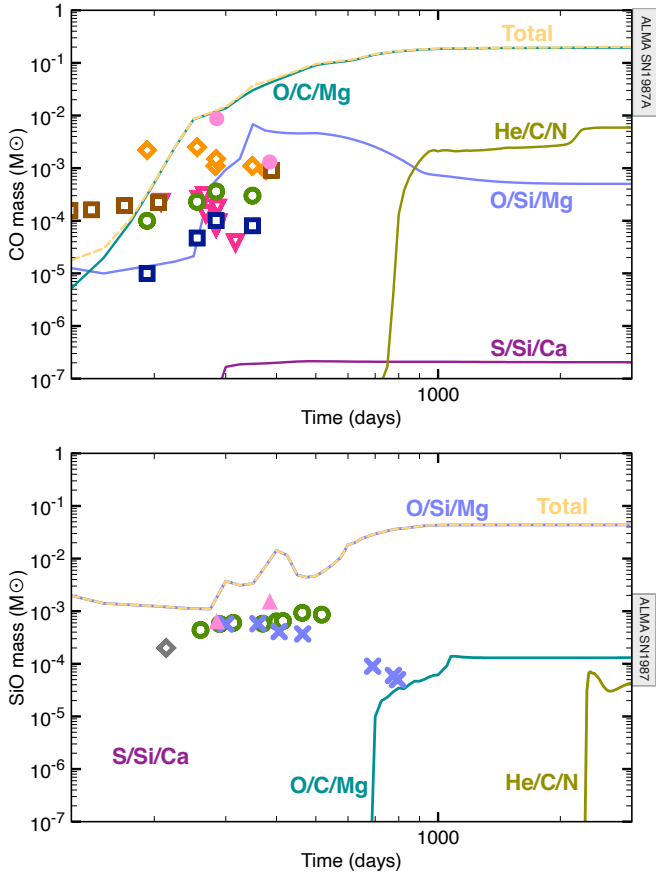


Fig. 20. Total CO and SiO masses and masses formed per region as a function of time for the standard case and available observations for various Type II SNe. Top: CO, where the brown empty square is SN2017eaw (Rho et al. 2018; Tinyanont et al. 2019), fuchsia empty triangle is SN2023ixf (Park et al. 2025), dark blue empty square is SN1987A (Spyromilio et al. 1988), green empty circle and orange empty rhombus are SN1987A for the LTE and NLTE case, respectively (Liu et al. 1992), pink circle is SN2024ggi (Mera et al. 2026). Bottom: SiO, where the dark grey empty rhombus is SN2005af (Kotak et al. 2006), green empty circle is SN1987A for NLTE (Liu & Dalgarno 1994), lavender cross is SN2004et (Kotak et al. 2009), pink triangle is SN2024ggi (Mera et al. 2026). Value ranges for both CO and SiO derived from ALMA data of SN1987A by Matsuura et al. (2017) are also indicated with filled grey rectangles.

data from combustion, aerosol and atmospheric chemistry. As already mentioned, further studies proved some proposed chemical routes were unlikely, e.g. for silicates (Bromley et al. 2016; Kimura et al. 2022). Regarding carbon clusters, the chemistry mainly relied on a unique study by Clayton et al. (1999) at a time when the structures of small carbon clusters were not well identified. They considered a very simple carbon chemistry unconnected with other species apart from atomic oxygen. Most processes were temperature-independent and their scheme for carbon cluster growth relied on chemical pathways with no energy barriers E_a and with large A factors (\equiv the reactions were fast – see Equation (16)). Such processes guaranteed an artificially efficient formation of carbon clusters in the ejecta over time and the whole temperature span.

Although it is difficult to directly compare results from the present study with those of existing investigations since the chemistry and the physical models are different, we can nevertheless outline some differences and drawbacks in recent inves-

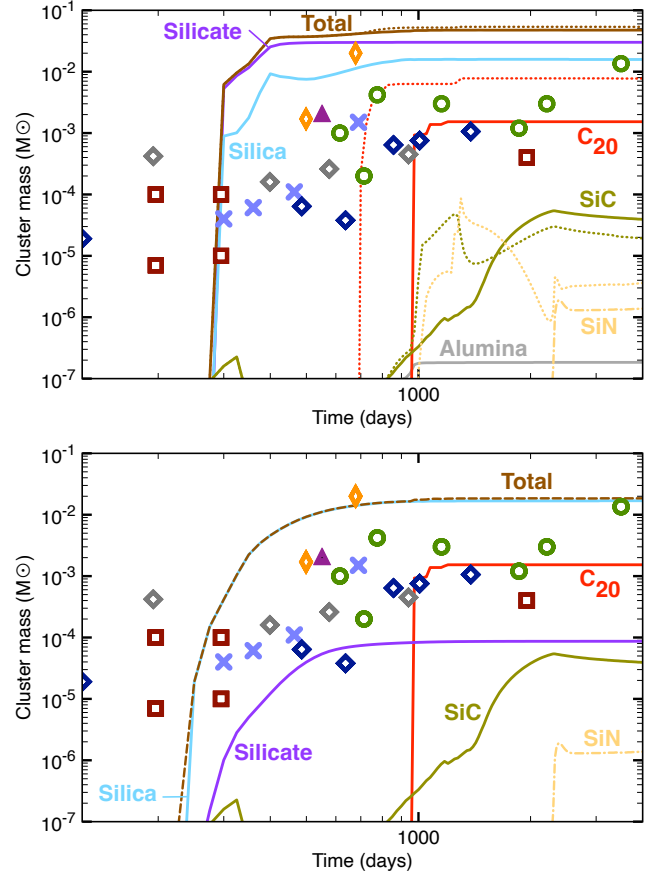


Fig. 21. Total dust cluster masses as a function of post-explosion time. Top: full lines show the standard case and dotted lines the standard case with a high density He/C/N region (see Sect. 4.5 for details). Bottom: Standard case with a low-temperature O/Si/Mg region (see Sect. 4.6 for details). Available observational data on dust are also represented for a number of Type IIP SNe: brown empty square is SN2017eaw (Shahbandeh et al. 2023), lavender cross is SN2004et (Fabbri et al. 2011), grey empty rhombus is SN2005af (Szalai & Vinkó 2013), green empty circle is SN1987A (Wesson et al. 2015; Bevan & Barlow 2016), orange empty rhombus is SN2003gd (Sugerman et al. 2006), dark blue empty rhombus is SN2011ja (Andrews et al. 2016; Tinyanont et al. 2016), purple triangle is SN2006bc (Gallagher et al. 2012).

tigations. Regarding the study of Sarangi & Cherchneff (2013) who model a SNe with a $15 M_{\odot}$ progenitor and a smaller ^{56}Ni mass ($^{56}\text{Ni} = 0.075 M_{\odot}$), we find the new chemical scheme is more efficient at forming molecules and dust clusters despite initial gas densities at day 100 that are lower by a factor of 100. Sarangi & Cherchneff find at day 1500 a molecular mass of 29.4% and a dust mass of 1.6% the ejecta mass when we have 39.95% and 2% for molecule and cluster masses, respectively. We also find a different composition of dust clusters: the dust composition in Sarangi & Cherchneff (2015) is mainly made of carbon, alumina, and silicates in order of decreasing mass, whereas this new model has a dust cluster composition dominated by silicates and silica, with small amount of alumina and eventually carbon clusters that form in high-density clumps. As for SiC and SiN, we might expect small masses of SiC and Si_3N_4 clusters to form in these carbon-rich, dense clumps, with SiC clusters always more abundant than those of Si_3N_4 by a few orders of magnitude. The present SiC mass at day 4000 for the standard case agree with the SiC dust mass derived at day 2000 by Sarangi & Cherchneff (2015). More generally, the SiC and

SiN results are consistent with the finding of meteorite studies where rare Si_3N_4 and SiC grains are isolated with both isotopic anomalies pointing to a common Type II SN origin (Nittler et al. 1995). Finally, we do not form small clusters of pure Si, Mg, and Fe in the inner Si/S/Ca region any longer, because of the low dimerisation rates we use in line with the low rates for SiO dimerisation. Therefore, the new chemistry tends to optimise molecular and dust formation in the ejecta despite a larger ^{56}Ni content and lower gas densities.

In his study of SN1987A, Sarangi (2022) uses the chemical model of Sarangi & Cherchneff (2013) and the coagulation formalism of Sarangi & Cherchneff (2015) applied to a SN with a $19M_{\odot}$ progenitor. The study provides a dust composition made of silicate, alumina, carbon and silicon carbide, in order of decreasing masses, with the carbon dust synthesis occurring at ~ 2500 days. As mentioned above, the scheme for carbon cluster growth guarantees an artificially efficient formation of carbon clusters over time, even at low gas temperature. At ~ 2500 days, the gas densities are \sim a few $1 \times 10^6 \text{ cm}^{-3}$ and the gas temperature is $\sim 100 \text{ K}$ according to Sarangi (2022). The rapid coagulation of carbon clusters into carbon dust at very late times seems extremely unlikely under these ejecta conditions. Indeed, our results show no carbon clusters in the form of large rings that could act as coagulation seeds, do form (e.g. C_{20}) for low gas densities; except for small carbons chains according to the low-temperature chemical pathways provided by Loison et al. (2014). Therefore, the very late carbon dust formation in SN1987A presented by Sarangi (2022) and the resulting infrared emission spectra need serious reconsideration.

Finally, Sluder et al. (2018) revisited studies by Sarangi & Cherchneff (2013, 2015) by investigating dust synthesis in a SN with a $20M_{\odot}$ progenitor and using a similar chemistry, an exhaustive description of dust growth including accretion and destruction processes, and a three-phase ejecta corresponding to low-density nickel bubbles, high-density shells of material swept up by the expanding bubbles, and an intermediate density region unaffected by the bubbles. Although we cannot directly compare results of both studies since the initial elemental compositions of the ejecta are different, we notice they derive temperature profiles quite different from those used by Sarangi (2022) and in this study. Furthermore, our standard case has a gas density at day 100 similar to their intermediate density region, while our high-density case for the C-rich outer region is similar to their shell density. The dust mass they obtained for their ambient phase is larger than ours by a factor of 10, while the dust composition is made of magnesia, iron sulphide, and pure silicon grains, in total contrast with our derived composition. Similarly, they found a dust mass larger than ours by a factor of 10 in their shell phase, again with a totally different chemical composition including silicon, magnesia and forsterite dust. It is unclear whether this large discrepancy in dust masses can be attributed to considering accretion at the surface of dust grains since the authors did not compare the results of cases with and without accretion in their study.

7. Summary and conclusions

In this paper, we present a new exhaustive model for the chemistry at work in the expanding ejecta of a non-interactive SN with progenitor mass of $15M_{\odot}$. We focus on the formation of molecules and dust clusters until ~ 11 years post-explosion and propose new chemical routes to silicate and carbon dust synthesis. One unique and exhaustive chemical scheme is applied to

all regions in the ejecta. By doing so, we removed the artificial chemical selection resulting from using a specific scheme for each region, as done in existing models. We tested the impact of clumps and gas molecular cooling on the model and highlight the following outcomes:

(1) Existing models are based on a silicate formation scheme involving the dimerisation of SiO as a first step, which artificially depletes the SiO content. Such a depletion is not seen in SN1987A. Furthermore, it was shown the dimerisation of SiO was extremely slow and inefficient for the ejecta conditions, thus invalidating these models. The new proposed scheme for silicate formation is efficient at forming dust clusters essentially in the inner oxygen core and represents a major improvement to existing models since SiO is just partially depleted in the dust formation process, in better agreement with observations,

(2) The ejecta has a large molecular component corresponding to $\sim 40\%$ of its mass while the dust represents $\sim 2\%$. The most abundant species are, in order of decreasing masses, O_2 , CO, SiS, SiO, CO_2 , SO_2 , CaS, N_2 , and CS. However, these molecules form in different ejecta regions. For example, SiS is typical of the inner ejecta, C_3 and N_2 formation peaks in the outer ejecta, while SO_2 forms in the inner oxygen core and CO and CO_2 in the outer oxygen core. The CO and SiO molecules form all over the ejecta with a peak in the outer and inner oxygen core, respectively. The SiO distribution is patchier than that of CO.

(3) We show carbon dust clusters need over-densities or clumps to form in the outer part of the ejecta, while low temperatures in the oxygen core are not conducive to the synthesis of silicates but favour the formation of silica. Cooling by SiO in the silicate-forming region could be further investigated to better model the temperature dependence of this region. We find the molecules CS, CN, and C_3 are tracers of gas conditions in the outer ejecta region,

(4) The exotic P- and F-bearing molecules form in small amounts in the oxygen core and the carbon-rich outer region, respectively. Only two species, PO and NF, have final masses of or above $1 \times 10^{-8} M_{\odot}$ at day 4000,

(5) Finally, our results show that any dust directly formed in the ejecta does so a few hundred days after explosion since the chemistry requires high enough gas temperatures and densities to proceed efficiently. The final total dust cluster mass is $\sim 1.7 \times 10^{-2}$ for our standard case considering a low-temperature profile mimicking the impact of SiO cooling in the O/Si/Mg region and $\sim 5.3 \times 10^{-2}$ considering our standard case and a high-density He/C/N region. This value range puts a stringent limit to the total dust mass that forms within the ejecta when surface deposition processes are not considered.

In a forthcoming paper, we will address the formation, growth, and time evolution of dust in SNe for various progenitor masses. We will aim to derive budgets for molecules and dust obtained with our new physico-chemical model of Type IIP SNe.

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Appendix A: Additional tables and figures.

Table A.1. Processes considered in the chemical model for Type II-P SN ejecta (adapted from [Biscaro & Cherchneff \(2014\)](#)).

		Reaction description			Gas regime/location
THERMAL					
Bimolecular	AB + C	→	BC + A	Neutral exchange	High temperature
	A + B	→	AB + hν	Radiative association	T independent
	AB + M	→	A + B + M	Collision dissociation	High density
	AB ⁺ + C	→	BC ⁺ + A	Ion–Molecule	T independent
	AB ⁺ + C	→	AB + C ⁺	Charge exchange	T independent
	A ⁺ + e ⁻	→	A + hν	Radiative recombination	T independent
	AB ⁺ + e ⁻	→	A + B	Dissociative recombination	T independent
Termolecular	A + B + M	→	AB + M	Three-body association	High density
NON-THERMAL					
	A + CE	→	A ⁺ + e ⁻ + CE	Ionisation by Compton e ⁻	Entire SN ejecta
	AB + CE	→	A + B + CE	Dissociation by Compton e ⁻	Entire SN ejecta
	AB + CE	→	A ⁺ + B + e ⁻ + CE	Ionisation by Compton e ⁻	Entire SN ejecta
	AB + CE	→	A + B ⁺ + e ⁻ + CE	Ionisation by Compton e ⁻	Entire SN ejecta

Table A.2. Absolute energies at $T = 0$ K calculated at the DFT - B3LYP/6-31G(d) level (in Hartree)^a.

Species	E	Species	E	Species	E
SiO ₃	-515.06253	MgO ₂	-350.38592	Mg ₂ O	-475.40517
Mg ₂ O ₂	-550.64069	MgSiO ^b	-564.79813	MgSiO ₂	-640.10426
MgSiO ₃	-715.34519	Mg ₂ SiO ₂	-840.22978	Mg ₂ SiO ₃	-915.52110
Mg ₂ SiO ₄ ^b	-990.77914				

Notes. ^(a) Absolute energies are corrected for the zero-point energies; ^(b) Calculation is from [Goumans & Bromley \(2012\)](#).

Table A.3. Final masses of molecules and dust clusters (in M_{\odot}) at day 4000 for various ejecta scenarios.

Species/Region	O/Si/Mg (Low T) ^a	He/C/N (High D) ^b	Total ejecta ^c
Detected molecules ^d			
CO	1.66×10^{-3}	4.09×10^{-3}	2.03×10^{-1}
SiS	9.25×10^{-3}	2.09×10^{-5}	5.01×10^{-2}
SiO	5.46×10^{-2}	1.07×10^{-4}	5.49×10^{-2}
SO ₂	1.22×10^{-2}	–	1.23×10^{-2}
CS	2.19×10^{-10}	5.28×10^{-4}	5.16×10^{-4}
SO	6.45×10^{-4}	4.28×10^{-6}	6.94×10^{-4}
Potentially detectable molecules ^d			
O ₂	4.52×10^{-1}	3.31×10^{-4}	5.74×10^{-1}
CO ₂	1.08×10^{-2}	8.38×10^{-4}	3.26×10^{-2}
C ₃	–	1.22×10^{-3}	2.45×10^{-2}
CaS	1.58×10^{-3}	4.00×10^{-7}	4.84×10^{-3}
N ₂	–	4.08×10^{-3}	2.77×10^{-3}
MgS	7.52×10^{-5}	4.46×10^{-6}	8.76×10^{-5}
CN	–	1.70×10^{-3}	4.23×10^{-4}
Al ₂ O	2.24×10^{-5}	–	2.35×10^{-5}
PO	1.76×10^{-6}	–	1.87×10^{-6}
FeS	2.33×10^{-8}	1.12×10^{-7}	3.87×10^{-5}
FeO	1.32×10^{-6}	4.03×10^{-7}	2.07×10^{-6}
SiO ₂	3.50×10^{-8}	6.67×10^{-8}	7.24×10^{-8}
NF	–	–	9.92×10^{-9}
NO	–	1.01×10^{-7}	1.05×10^{-10}
Total mass	5.74×10^{-1}	1.29×10^{-2}	9.33×10^{-1}
Dust clusters ^d			
Mg ₂ Si ₂ O ₆ - enstatite	8.76×10^{-5}	–	8.76×10^{-5}
Mg ₄ Si ₂ O ₈ - forsterite	1.02×10^{-7}	–	1.05×10^{-7}
Si ₃ O ₅ - quartz	1.48×10^{-2}	–	1.48×10^{-2}
Si ₃ O ₆ - quartz	2.04×10^{-3}	–	2.04×10^{-3}
Al ₄ O ₆ - alumina	4.01×10^{-12}	–	1.94×10^{-10}
C ₂₀ - carbon	–	7.73×10^{-3}	7.73×10^{-3}
SiC - silicon carbide	2.04×10^{-11}	1.58×10^{-5}	3.56×10^{-5}
SiN - silicon nitride	7.22×10^{-13}	3.61×10^{-6}	1.38×10^{-6}
Total mass	1.69×10^{-2}	7.75×10^{-3}	1.70×10^{-2}

Notes. ^(a) Masses produced by a low-temperature O/Si/Mg region - see Sect. 4.6; ^(b) Masses produced by a high-density He/C/N region - see Sect. 4.5; ^(c) Masses summed over the Si/S/Ca, O/C/Mg, and He/C/N regions of Table 5 and the low-temperature O/Si/Mg region as given by 1st column of this table; ^(d) Masses less than $10^{-13} M_{\odot}$ are labelled as –.

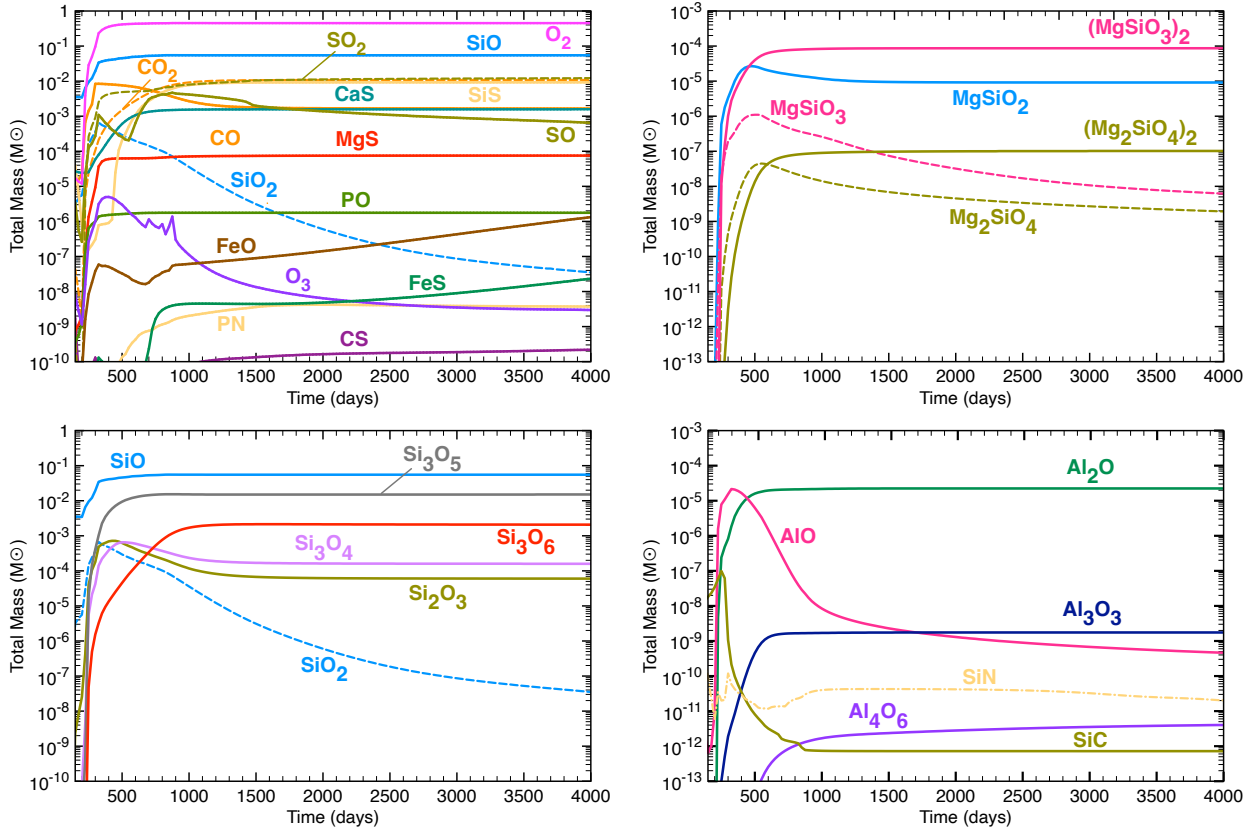


Fig. A.1. Total mass of molecules and dust clusters produced in the O/Si/Mg region as a function of post-explosion time for the low-temperature case discussed in Sect. 4.6. Top-left: Molecules. Top-right: Silicates. Bottom-left: Silica. Bottom-right: Alumina.